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DOE/PC/90015--T9

PRODUCTI OF JET FUEL FROM COAL-DERIVED LI DS

Report No. 15

DOE/PC/90015--T9

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TECHNICAL STATUS

This technical report is being transmitted in advance of DOE review, and no further dissemination or publication will be made of the report without prior approval of the DOE Project/Program Manager.

EXECUTIVE SUMMARY

Amoco and Lummus Crest, under a contract with the United States Department of Energy, are evaluating the process options and economics for upgrading the naphtha, crude phenols, and tar oil by-products from the Great Plains Coal Gasification Plant to jet fuels and other salable products. Analytical characterizations of these three by-products indicate the range of products that can be manufactured from each, and potential problems which could be encountered during refining. These characterizations, along with limited experimental data and Amoco's proprietary process models, were used to design conceptual processing schemes for maximizing the production of Grades JP-4, JP-8, and high-density (JP-8X) jet fuels from the by-product liquids. These conceptual designs have been forwarded to Lummus Crest, Inc. for process design and integration with the existing Great Plains plant. The first two cases are now complete. In addition to the maximum jet fuel schemes, conceptual designs have also been formulated for maximizing profits from refining of the Great Plains by-products. Conceptual processing schemes for profitable production of JP-4, JP-8, and JP-8X have been developed, as has a "maximum profit" case. All four of these additional cases have now been transferred to Lummus for design and integration studies. Development of these schemes required the use of linear programming technology. This technology includes not only conventional refining processes which have been adapted for use with coal-derived liquids (e.g. hydrotreating, hydrocracking), but also processes which may be uniquely suited to the Great Plains by-products such as cresylic acid extraction, hydrodealkylation, and needle coking. Future work will include experimental confirmation of these preliminary designs.

BACKGROUND

The goal of the national energy policy is to foster an adequate supply of energy at reasonable costs. The United States supplies only about 60% of its petroleum needs from domestic production, and the outlook for domestic and world supply and demand is not reliable over the long term considering price fluctuations and supply based on conventional fuel supplies alone. Synthetic liquid fuels are an essential part of an energy scenario which provides the United States with the means, when required, to reduce reliance on imported petroleum. As a consequence, research is being conducted into better ways of obtaining environmentally acceptable synthetic liquid fuels from alternative sources such as coal.

A significant portion of the United States demand for liquid fuels is the requirement by the Department of Defense (DOD). The DOD accounts for approximately 2.7% of the nation's petroleum consumption, including approximately 240,000 barrels per day of aviation turbine fuel (Grade HP-4) used by the Air Force. JP-4 is a naphtha-based fuel used mainly in the United States, while overseas the Air Force uses a kerosene-type fuel, Grade JP-8. Because of the need to assure adequate supplies of either turbine fuel at acceptable costs, and in view of the uncertain outlook for petroleum, the Air Force has investigated the characteristics, cost, and yield of aviation fuels produced from tar sands, shale oil, and heavy oils and is seeking similar data for coal-derived liquids.

There are two main types of coal-derived liquids: those produced as the primary products of direct coal liquefaction and those produced as the by-products of coal pyrolysis to gaseous products. Currently, there are no commercial-scale direct liquefaction plants in the United States, but there is a commercial-scale pyrolysis process, the Great Plains Gasification Plant in Beulah, North Dakota. This plant has a capacity to produce up to 160 million cubic feet per stream-day of high-BTU methane from North Dakota lignite. The plant generates three liquid streams as by-products, tar oil, crude phenol, and naphtha; their production rates are approximately 3,300, 900, and 750 barrels per day, respectively. All three streams are available as potential aviation turbine fuel, either JP-4 or JP-8, for the Air Force. The streams are currently burned for plant fuel.

Because the Great Plains Gasification Plant (GPGP) is in close proximity to several Air Force bases along our northern tier, these three by-product streams represent a potential indigenous and nearby supply of fuel. In particular, the Air Force base at Minot, North Dakota, is quite remote from aviation turbine fuel supplies and could especially benefit from this development if an aviation turbine fuel produced at the Great Plains Gasification Plant were compatible with aircraft systems and cost-competitive with other supplies. In addition, a long-range strategic objective of the Air Force is the development of a high-density aviation turbine fuel. Such a fuel is attractive because of its higher energy content per unit volume, which could extend the range of an aircraft limited by the size of its fuel tank. Because of their aromaticity, coal liquids are ideal feedstocks for the production of high-density fuels.

In view of these considerations, the Department of Energy and the Department of Defense have a joint program to assess the technical and economic

feasibility for producing aviation turbine fuel from the by-product streams of GPCP. These streams, as well as fractions thereof, will be characterized subsequently processed over a wide range of conditions. The resulting turbine fuel products will be analyzed to determine their chemical and physical characteristics as compared with petroleum-based fuels to meet the military specification requirements. Since no fixed performance specifications currently exist for a high-density turbine fuel, reaction products and intermediates will only be characterized to indicate the feasibility of producing such a fuel. In addition, to the extent that portions of the three by-product streams are not suitable for aviation turbine fuel production, the technical and economic feasibility of co-producing other products such as motor gasoline and petrochemicals will be assessed in an effort to improve the economic viability of the Great Plains Gasification Plant.

PROGRAM OBJECTIVES

The goal of this program is to investigate the potential of producing aviation turbine fuels, as well as other potentially marketable products, from the tar oil, crude phenol, and naphtha streams available at the Great Plains Gasification Plant. The specific objectives to meet this goal include determination of the cost, yield, chemical properties, and physical characteristics of aviation turbine fuels, etc., which can be produced from tar oil, crude phenol, and naphtha using commercially available, licensable technology. The technology will be selected and designed for integration at Great Plains based on the program described here. The process technology selected will depend on relative technical merit as well as economic and strategic factors. Economically, emphasis will be placed upon minimizing both operating cost and capital investment. Strategically, a process that possesses the flexibility for changing the product slate based on market conditions is desirable. Many process schemes can simultaneously satisfy these requirements. Identification of all practical schemes; ranking of their relative attractiveness based upon technical, economic, and strategic merit; experimental confirmation of selected process schemes; and a detailed process design of a preferred process will be provided. Possible facilities for a commercial-scale (10,000 barrels) production test will be sought at the end of the project.

PROJECT DESCRIPTION

As shown in Figure 1, this project is divided into five major tasks. The first task, Process Concept Definition, includes three subtasks: Feedstock Analysis, Process Modeling and Design, and Economic Modeling. The first of these subtasks, Feedstock Analysis, involves analytical characterizations of samples of each by-product taken at six-week intervals. The results from this program, which provide an indication of the average quality of each stream and the variability of that quality over time, are an important input to the second subtask, Process Modeling and Design. Other inputs to this subtask include limited experimental processing data on the Great Plains by-products and similar coal liquids, Amoco's petroleum refining process models and linear programming technology, and Lummus' process simulation and design programs. The major objective of this subtask is to produce six conceptual designs for facilities to refine the Great Plains by-products. These six designs are

listed in Figure 2. They include designs for maximizing production of each grade of jet fuel (JP-4, JP-8, JP-8X) as well as designs for maximizing profits while producing each of the jet fuel grades. In addition, we have provided a seventh case for "maximum profit" from the by-products. Once the conceptual designs are completed by Amoco and Lummus, they will be subjected to a discounted cash flow rate of return (DCFROR) analysis (Subtask 1.3).

The two products from Task 1 will be the design and economic results for each of the six designs and a plan for bench scale testing (Task 2) to confirm any assumptions made in Task 1. Based on the design and economic results from Task 1 and the experimental results from Task 2, the Department of Energy and the Department of Defense will decide on a preferred processing scheme for the Great Plains liquids. Amoco will then carry out pilot plant testing (Task 3) to confirm the process design and to provide barrel quantities of product for testing by the government. The pilot plant results will be used by Amoco and Lummus to develop a preliminary process design (Task 4) for a plant to upgrade the liquid by-products at Great Plains. Finally, in Task 5, Lummus will locate existing facilities where the processing scheme can be carried out on a scale sufficient to provide jet fuel for aircraft testing.

RESULTS AND DISCUSSION

During this quarter conceptual design cases were developed for maximizing profit from the liquid by-products from Great Plains and for profitable production of each of three aviation turbine fuels: JP-4, JP-8, and JP-8X. All four of these cases required linear programming technology to design the optimum processing configurations. In addition, during this quarter Lummus Crest, Inc. completed process designs and integration with the Great Plains plant for maximum production of JP-4 and JP-8.

Case 7: "Maximum Profit" Case

The process design basis for the conceptual commercial plant which generates the maximum profit from the Great Plains liquid by-products has been developed by our linear programming model. The properties of these by-products are the same as reported in the JP-4, JP-8, and JP-8X cases. This maximum profit case limits sales of o-cresol, m- and p-cresol, xylenols, and cresylic acids to 10% of the United States market, and profitability is very sensitive to this assumption.

Process Block Flow Diagram.--Figure 3 shows the process units needed and the quantities processed in barrels per calendar day (BCD). Additional properties of the streams are given in Table I. The Great Plains crude phenol stream is extracted in a Phenoraffin unit to provide a stream of purified phenols for sale. It also provides 242 BCD of cresylic acids, of which 138 BCD are sold. The remaining 103 BCD are fractionated to make 21 BCD of o-cresol, 53 BCD of m-, p-cresol, and 30 BCD of xylenols. The by-product neutral oil stream (267 BCD) from the Phenoraffin unit is routed to the Great Plains liquid fuels pool.

The tar oil stream is also routed to fuel. This is consistent with current Great Plains plant operations.

The Great Plains naphtha is distilled to remove the 160-°F fraction. This fraction is unacceptable hydrotreater feed because of its high heteroatom (especially oxygen) content. This 160-°F stream is sent to the plant liquid fuel pool. It may be possible to eliminate this distillation step if operations of the existing Great Plains naphtha stripper can be improved to eliminate the impurities there.

The 160+°F stream (476 BCD) is hydrotreated to reduce the moderate levels of heteroatom impurities in it before being processed in an aromatics recovery unit. It is possible that this hydrotreating may not be necessary, but a conservative approach was taken for this process design basis. Elimination of the hydrotreating step would raise the profit from this case. The 430 standard cubic feet per barrel (SCFB) of hydrogen for the hydrotreating step is obtained from the Great Plains syngas stream with a PSA unit.

The naphtha aromatics recovery unit produces 287 BCD of benzene, 89 BCD of toluene, and 13 BCD of xylene for sales. The aromatics recovery unit also produces 54 BCD of a gasoline blending stock from 19 BCD of light raffinate, 12 BCD of heavy raffinate, and 13 BCD of toluene. These streams are not shown separately since they can be blended within the process unit battery limits. If this blending stock is combined with 8 BCD of purchased normal butane, 62 BCD of salable unleaded regular gasoline result. Properties of the finished gasoline are shown in Table II.

Process Conditions and Utilities.--The process conditions for the PSA, Phenoraffin, and naphtha aromatics recovery units will have to be obtained from process vendors. A preliminary, estimated utilities balance for the units in the maximum profit case are shown in Table III.

Case 2: Profitable JP-4 Production

Figure 4 shows the process units needed and the quantities processed in barrels per calendar day (BCD) for the profitable case which produces some JP-4. The Great Plains crude phenol stream is extracted in a Phenoraffin unit to provide a stream of purified phenols for sale. It also provides 242 BCD of cresylic acids, of which 138 BCD are sold. The remaining 103 BCD are fractionated to make 21 BCD of o-cresol, 53 BCD of m-, p-cresol, and 30 BCD of xylenols. The by-product neutral oil stream (267 BCD) from the Phenoraffin unit is routed to the Great Plains liquid fuels pool.

The tar oil stream is hydrotreated at the same conditions as in the maximum JP-4 case. The 160°F- cut is sent to gasoline blending, the 160-500°F cut is blended to JP-4, and the 500°F+ is hydrocracked. The hydrocracker produces 232 BCD of 160°F- naphtha and 1255 BCD of JP-4 blending stock.

The Great Plains naphtha is distilled to remove the 160°F- fraction. This fraction is unacceptable hydrotreater feed because of its high heteroatom (especially oxygen) content. This 160°F- stream is sent to the plant liquid fuel pool. It may be possible to eliminate this distillation step if operations of the existing Great Plains naphtha stripper can be improved to eliminate the impurities there.

The 160°F+ stream (476 BCD) is hydrotreated to reduce the moderate levels of heteroatom impurities in it before being processed in an aromatics recovery

unit. It is possible that this hydrotreating may not be necessary, but a conservative approach was taken for this process design basis. Elimination of the hydrotreating step would raise the profit from this case. The 430 standard cubic feet per barrel (SCFB) of hydrogen for the hydrotreating step is obtained from the Great Plains syngas stream with a PSA unit.

The naphtha aromatics recovery unit produces 212 BCD of benzene, 75 BCD of toluene, and 10 BCD of xylene for sales. The aromatics recovery unit also produces 31 BCD of a gasoline blending stock from 22 BCD of light raffinate and 9 BCD of heavy raffinate. These streams are not shown separately since they can be blended within the process unit battery limits.

Case 4: Profitable JP-8 Production (Preliminary)

Figure 5 shows the process units needed and the quantities processed in barrels per calendar day (BCD) for the profitable case which produces some JP-8. The Great Plains crude phenol stream is extracted in a Phenoraffin unit to provide a stream of purified phenols for sale. It also provides 242 BCD of cresylic acids, of which 138 BCD are sold. The remaining 103 BCD are fractionated to make 21 BCD of o-cresol, 53 BCD of m-, p-cresol, and 30 BCD of xylenols. The by-product neutral oil stream (267 BCD) from the Phenoraffin unit is routed to the Great Plains liquid fuels pool.

The tar oil stream is hydrotreated at the same conditions as in the maximum JP-8 case. The 300°F- cut is sent to gasoline blending, the 300-550°F cut is blended to JP-8, and the 550°F+ is hydrocracked. The hydrocracker produces 469 BCD of 300°F- naphtha and 460 BCD of JP-8 blending stock.

The Great Plains naphtha is distilled to remove the 160-°F fraction. This fraction is unacceptable hydrotreater feed because of its high heteroatom (especially oxygen) content. This 160-°F stream is sent to the plant liquid fuel pool. It may be possible to eliminate this distillation step if operations of the existing Great Plains naphtha stripper can be improved to eliminate the impurities there.

The 160+°F stream (476 BCD) is hydrotreated to reduce the moderate levels of heteroatom impurities in it before being processed in an aromatics recovery unit. It is possible that this hydrotreating may not be necessary, but a conservative approach was taken for this process design basis. Elimination of the hydrotreating step would raise the profit from this case. The 430 standard cubic feet per barrel (SCFB) of hydrogen for the hydrotreating step is obtained from the Great Plains syngas stream with a PSA unit.

The naphtha aromatics recovery unit produces 287 BCD of benzene, 89 BCD of toluene, and 13 BCD of xylene for sales. The aromatics recovery unit also produces 54 BCD of a gasoline blending stock from 29 BCD of light raffinate, 12 BCD of heavy raffinate, and 13 BCD of toluene. These streams are not shown separately since they can be blended within the process unit battery limits. This blending stock is combined with the hydrotreater and hydrocracker naphtha streams to make salable gasoline and naphtha streams.

Case 6: Profitable JP-8X Production (Preliminary)

Figure 6 shows the process units needed and the quantities processed in barrels per calendar day (BCD) for the profitable case which produces some JP-8X. The Great Plains crude phenol stream is extracted in a Phenoraffin unit to provide a stream of purified phenols for sale. It also provides 242 BCD of cresylic acids, of which 138 BCD are sold. The remaining 103 BCD are fractionated to make 21 BCD of o-cresol, 53 BCD of m-, p-cresol, and 30 BCD of xyenols. The by-product neutral oil stream (267 BCD) from the Phenoraffin unit is routed to hydrotreating with 2469 BCD of GP tar oil.

Some (427 BCD) tar oil is routed to liquid fuels with the rest hydrotreated at the same conditions as in the maximum JP-8X case. The 300°F- cut is sent to gasoline blending, the 300-550°F cut is blended to JP-8X, and the 550°F+ is sent to fuel.

The Great Plains naphtha is distilled to remove the 160°F- fraction. This fraction is unacceptable hydrotreater feed because of its high heteroatom (especially oxygen) content. This 160°F- stream is sent to the plant liquid fuel pool. It may be possible to eliminate this distillation step if operations of the existing Great Plains naphtha stripper can be improved to eliminate the impurities there.

The 160°F+ stream (476 BCD) is hydrotreated to reduce the moderate levels of heteroatom impurities in it before being processed in an aromatics recovery unit. It is possible that this hydrotreating may not be necessary, but a conservative approach was taken for this process design basis. Elimination of the hydrotreating step would raise the profit from this case. The 430 standard cubic feet per barrel (SCFB) of hydrogen for the hydrotreating step is obtained from the Great Plains syngas stream with a PSA unit.

The naphtha aromatics recovery unit produces 287 BCD of benzene, 102 BCD of toluene, and 13 BCD of xylene for sales. The aromatics recovery unit also produces 41 BCD of a gasoline blending stock from 29 BCD of light raffinate and 12 BCD of heavy raffinate. These streams are not shown separately since they can be blended within the process unit battery limits.

Process Design Description, Case 1, Maximum JP-4 Production

Lummus Crest, Inc. has developed a design basis and process economics for Case 1, the maximum JP-4 case. The process design description, excerpted from Lummus' preliminary report, is given in Appendix A. The complete design and economics of Case 1 will be given in the final, approved Task 1 report which will be issued after all seven design cases are completed.

Economically, this preliminary analysis shows that manufacturing 4050 BCD of JP-4 would require a capital investment of \$53MM and would lower the Great Plains profitability approximately \$1.2MM per year.

Process Design Description, Case 3, Maximum JP-8 Production

Lummus Crest, Inc. has developed a design basis and process economics for Case 3, the maximum JP-8 case. The process design description, excerpted from Lummus' preliminary report, is given in Appendix B. The complete design and

economics of Case 3 will be given in the final, approved Task 1 report which will be issued after all seven design cases are completed.

Economically, this preliminary analysis shows that manufacturing 2320 BCD of JP-8 would require a capital investment of \$53MM and would lower the Great Plains profitability approximately \$5.9MM per year.

CONCLUSIONS AND FUTURE WORK

Based upon analytical characterizations and conceptual design studies, the conversion of the Great Plains liquid by-products to jet fuels appears to be technically feasible. The design bases for conceptual process plants to maximize profitability and to produce Grades JP-4, JP-8, or high-density jet fuel (JP-8X) profitably have been completed and transmitted to Lummus Crest, Inc. for detailed design and integration with the existing Great Plains plant. Lummus has completed preliminary designs for maximized production of JP-4 and JP-8.

In the future the plant designs and economic evaluations will be completed. At that point bench-scale experiments will be performed to test assumptions made during this conceptual design phase. The results from the design and economic evaluations and the bench-scale experiments will provide the United States Department of Energy and Department of Defense with sufficient information to decide on a preferred processing scheme for further testing and evaluation by Amoco and Lummus Crest.

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TABLE I
MAXIMUM PROFIT CASE STREAM PROPERTIES

<u>Property</u>	<u>GP Phenol</u>	<u>Tar Oil</u>	<u>GP Naph</u>	<u>Hydro- gen</u>	<u>Sales Phenol</u>	<u>Cres. Acid</u>
Volume, BCD	833	2896	660	-	283	242
API Gravity	1.6	6.6	39.6	-	2.0	8.6
Weight, M#/cal.hr.	12.9	43.1	8.0	0.05	4.4	3.6
<u>Property</u>	<u>Neutral Oil</u>	<u>Pheno. Water</u>	<u>160-</u>	<u>160+</u>	<u>Wet Gas</u>	<u>Htrt. Naphtha</u>
Volume, BCD	267	42	184	476	36	444
API Gravity	0.7	1.5	61.0	33.0	-	34.0
Weight, M#/cal.hr.	4.2	0.7	2.0	6.0	0.5	5.5
<u>Property</u>	<u>Gasol. Stock</u>	<u>Butane</u>	<u>Sales Gasol.</u>	<u>Benzene</u>	<u>Toluene</u>	<u>Xylene</u>
Volume, BCD	54	8	62	287	89	13
API Gravity	26.0	110.6	58.1	28.5	30.8	30.6
Weight, M#/cal.hr.	0.6	0.1	0.7	3.7	1.1	0.2
<u>Property</u>	<u>o- Cresol</u>	<u>m-,p- Cresol</u>	<u>Xyle- nols</u>			
Volume, BCD	21	53	30			
API Gravity	5.9	5.9	14.4			
Weight, M#/cal.hr.	0.3	0.8	0.4			

TABLE II
UNLEADED REGULAR GASOLINE PROPERTIES

<u>Property</u>	<u>Estimated Quality</u>
Motor Octane	83.2
Research Octane	90.8
Reid Vapor Pressure, psi	12.7
Temperature for V/L=20, °F	164
Percent Distilled at 230°F	63
Percent Distilled at 300°F	83
Weight Percent Sulfur	.000
Specific Gravity	.746
API Gravity	58.1

TABLE III
ESTIMATED UTILITIES PER CALENDAR DAY

<u>Inputs</u>	<u>Fuel</u> <u>MMBtu</u>	<u>Cool.</u> <u>Water</u> <u>M Gal</u>	<u>Power</u> <u>KWH</u>	<u>Steam</u> <u>M Lb.</u>	<u>Proc.</u> <u>Water</u> <u>M Gal</u>	<u>Cat&</u> <u>Chem</u> <u>\$</u>
Purchases		193	4603	595	2	310
Hydrotreater Gas	124					
Liquid Stocks	20564					
<u>Process Units</u>						
Aromatic Recov.	-25	-35	-788	-150		-51
Phenoraffin		-75	-1666	-342		-250
Cresylic Acid Dist		-16	-383	-81		
Purchased C4 Dist	-1	-1	-4			
Naphtha Dist			-116	-16		
Naphtha Hydrotret	-39	-63	-411	-3	-1	-3
PSA			-1139			
Sulfur Plant	-3	-4	-96	-4	-1	-5
<u>Output</u>						
GP Fuel Pool	-20620					

FIGURE 1 PRODUCTION OF JET FUEL FROM COAL DERIVED LIQUIDS: AMOCO/LUMMUS ACTIVITIES

FIGURE 2

SUBTASK 1.2:
PROCESS MODELING
AND DESIGN CASE SUMMARY

THE FOLLOWING DESIGN CASES WILL RESULT FROM ACTIVITIES IN THIS
SUBTASK:

<u>CASE</u>	<u>DESCRIPTION</u>
1	MAXIMUM JP-4 PRODUCTION
2	MAXIMUM PROFIT PRODUCT SLATE INCLUDING JP-4
3	MAXIMUM JP-8 PRODUCTION
4	MAXIMUM PROFIT PRODUCT SLATE INCLUDING JP-8
5	MAXIMUM JP-8X PRODUCTION
6	MAXIMUM PROFIT PRODUCT SLATE INCLUDING JP-8X
7	MAXIMUM PROFIT SLATE

NOTE: CASES 2, 4, 6, AND 7 REQUIRE LINEAR PROGRAMMING
TECHNOLOGY.

FIGURE 3
GREAT PLAINS LIQUID BY-PRODUCTS USE
MAXIMUM PROFIT CASE

FIGURE 4

GREAT PLAINS LIQUID BY-PRODUCTS USE
PROFITABLE JP-4 CASE

FIGURE 5

GREAT PLAINS LIQUID BY-PRODUCTS USE PROFITABLE JP-8 CASE

FIGURE 6

GREAT PLAINS LIQUID BY-PRODUCTS USE
PROFITABLE JP-8X CASE

APPENDIX A

AMOCO/DOE

GREAT PLAINS GASIFICATION PLANT

JET FUEL FROM COAL DERIVED LIQUIDS

PROCESS DESIGN DESCRIPTION

CASE 1

MAXIMUM JP-4 PRODUCTION

SUBTASK 1.2

PRELIMINARY

LCI PROJECT 5571
DATE - DEC. 2, 1987

1.0 CASE DESCRIPTION

1.1 Overall Process Description

The purpose of this case is to maximize the production of type JP-4 aviation turbine fuel from Great Plains liquid by products. Figure 1 presents a block diagram for the process and referring to Figure 1 the flow is as follows:

Two by product streams are combined and charged to the hydrotreater (Area 100).

- Tar Oil 47620 #/hr (3182 BPSD)
- Phenol 14213 #/hr (920 BPSD)

The hydrotreater is a 3 stage expanded bed type process which removes 99% + of the sulfur, nitrogen, and oxygen compounds and begins the conversion of 500°F+ material. The hydrotreater adds a large quantity of hydrogen to the feed (3850 SCF/bbl) which results in a high heat of reaction. An expanded bed type reactor was chosen to both control and utilize the heat of reaction. Three stages were used to both control the temperature rise as well as to obtain the high efficiency associated with staging a back-mixed reactor.

The hydrotreater produces 6 streams:

- High pressure purge gas (approximately 90% hydrogen) which is sent to the Rectisol Unit in the SNG plant for recovery of the H_2 and CH_4 .
- Low pressure fuel gas (75 psig) which is sent to the main boiler in the SNG plant.
- Unstabilized naphtha which is sent to the combined naphtha stabilizer in the hydrocracker (area 200). After stabilization, to control vapor pressure, the naphtha is sent to the main boiler in the SNG plant.
- JP4 turbine fuel which is combined with JP4 produced in the hydrocracker (area 200) and sent to storage.
- 500°F+ unconverted bottoms product which is sent to the hydrocracker (area 200).
- Wastewater containing, NH_4OH and NH_4HS which is sent to the PHOSAM unit in the SNG plant for recovery of the H_2S and NH_3 .

- Approximately 750 #/day of spent catalyst which is shipped to a catalyst reclaimer in the same drums that the catalyst is received in.

The 500°F+ unconverted stream from the expanded bed hydrotreater (area 100) is charged to the fixed bed hydrocracker (area 200). The hydrocracker converts this material to naphtha and JP-4 turbine fuel. For this service a 5 stage unit was chosen with 65% conversion per pass. This unit also includes a naphtha stabilizer which stabilizes both the naphtha produced in the hydrotreater and hydrocracker.

The hydrocracker produces 4 streams in addition to JP-4.

- High pressure purge gas (approximately 90% hydrogen) which is sent to the Rectisol Unit of the SNG plant for recovery of the H₂ and CH₄.
- Low pressure fuel gas (75 psig) which is sent to the main boiler in the SNG plant.
- Stabilized naphtha which is sent to the main boiler in the SNG plant.
- A small sour water stream which is sent to the PHOSAM unit in the SNG plant or alternatively used as part of the injection water to the hydrotreating plant.

Hydrogen make-up for both the Hydrotreater and the Hydrocracker is supplied from a PSA Hydrogen Unit. High pressure (355 psig) synthesis gas from the Rectisol Unit (which contains about 63% hydrogen) is charged to the PSA unit which recovers 86% of the contained hydrogen as a high pressure 99.99% purity hydrogen gas product. The remaining purge gas is available at low pressure (5 psig) which has a fuel value of about 565 BTU/ft³. This H₂, CO & CH₄ rich gas is recompressed into the methanation unit of the SNG plant.

1.2 Overall Material Balance

The overall material balance is presented in Table 1.1 which presents overall material balances for the major process units. Detailed material balances for each unit can be found in appendixes A&B. The balance was computed on the basis that the fuel value of the feed will be replaced by fuel gas and naphtha produced in the process and the difference made up by the purchase of #6 Fuel Oil.

The overall balance is as follows:

Feeds

4109 BPSD of Tar Oil and Phenol Feed
3372 BPSD of #6 Fuel Oil
13.34 MMSCFD equivalent SNG product loss due to the syn gas feed to the PSA unit.

Products

4278 BPSD of JP-4 turbine fuel
8.53 MMSCFD Equivalent SNG product credit due to HDT, HDC & PSA purge gas reinjection into SNG Plant.

1.3 Overall Utility Balance

The overall utility consumption of the complex is as follows:

#6 Fuel Oil	3372 BPSD
SNG Equivalent	
of Syn Gas & Purge Gas	4.81 MM SCFD
Power	7100 kW
Cooling Water	2400 GPM (30°F rise)
Process Water	18.5 GPM

In addition the process exports 5280 #/hr of 100 psig saturated steam which was credited against boiler requirements.

Figure 1: Case 1 - Maximum JP-4 Production

Table 1.1 Great Plains Case 1: Maximum JP-4 Production

Tar Oil Feed====>	47620	#/hr	3187	BPBD
Phenol Feed====>	14213	#/hr	920	BPBD
Total Oil Feed====>	61833	#/hr	4102	BPBD
JP-4 Product====>	49985	#/hr	4276	BPBD
SNB Product Loss=>	8268	#/hr	4.8	MMBCPD
Fuel Oil Makeup=>	46646	#/hr	3772	BPBD

Expanded Bed Hydrotreater

Comp.	Wt %	Grav	#/hr	#Mole/hr	BPBD
Feeds					
H2	5.87		3631	1801.1	
Oil	100.00	1.0342	61833		4102
Total	105.87		65464		
Products					
Purge Gas	0.13		79	24.5	
Fuel Gas	2.13		1319	65.0	
Naphtha	5.50	0.7238	3403		323
JP-4	56.14	0.6203	35647		3008
SNB loss	27.51	0.9465	17056		1236
H2S in SW	11.06		6079	379.9	
H2O in SW	0.35		210	6.4	
NH3 in SW	0.97		601	35.4	
Total	105.87		65464		4554

Fixed Bed Hydrocracker

Comp	Wt %	Grav	#/hr	#Mole/hr	BPBD
Feeds					
H2	2.95		504	250.0	
SNB Feed	100.00	0.9465	17056		1236
Total	102.95		17560		
Products					
Purge Gas	0.21		36	10.3	
Fuel Gas	3.95		673	24.0	
Naphtha	16.49	0.6787	2813		284
JP-4	82.30	0.7563	14037		1273
H2S in SW	0.003		0.5	0.02	
NH3 in SW	0.003		0.5	0.03	
Total	102.96		17560		1558

Naphtha Stabilizer

Comp.	Wt %	Grav	#/hr	#Mole/hr	BPBD
HDT Nap	54.75	0.7238	3403		323
HCR Nap	45.25	0.6787	2813		284
Stab Nap	92.79	0.6890	5768		574
Fuel Gas	7.21		448	9.8	

PSA Hydrogen Recovery Unit (96% Recovery)

Component	H ₂	CO	CO ₂	C ₁ +C ₂	C ₂ H ₆	N ₂ +Ar	Total
Mol %							
Feed Gas	116.28	34.26	1.71	29.84	0.58	0.35	184.01
Prod. H ₂	100.00	0.01					100.01
Purge Gas	16.28	34.25	1.71	29.84	0.58	0.35	84.12
Wt %							
Feed Gas	116.28	475.91	55.44	237.46	8.63	5.55	900.71
Prod. H ₂	100.00	0.12	0.00	0.00	0.00	0.00	100.12
Purge Gas	16.28	475.83	55.44	237.46	8.63	5.55	800.19
#Mol/hr							
Feed Gas	2385.0	702.7	55.8	612.0	11.9	7.2	3774.6
Prod. H ₂	2051.1	0.2	0.0	0.0	0.0	0.0	2051.3
Purge Gas	333.9	702.5	55.8	612.0	11.9	7.2	1723.3
#Btu/hr							
Feed Gas	4003	19661	2458	9819	357	119	30780
Prod. H ₂	4173	5	0	0	0	0	4178
Purge Gas	673	19676	2458	9819	357	119	30710

Fuel Gas Generated in Hydrotreating and Hydrocracking

Component	#/hr	#Mol/hr	MMBTU/hr
HDTB FG Produced	1319	65.0	28.1
HCI FG Produced	673	24.0	12.1
Stab FG Produced	448	9.8	6.2
Total Fuel Gas	2440	98.9	46.0

Purge Gas Generated in PSA Hydrogen Unit

Component	#/hr	#Mol/hr	BTU/ft ³	MMBTU/hr
H ₂	673	333.9	324	41.0
CO	19676	702.5	321	85.5
CO ₂	2458	55.8	0	0.0
C ₁	9819	612.0	1010	234.3
C ₂	357	11.9	1769	8.0
N ₂ +Ar	229	7.2	0	0.0
Total	33212	1723.3	565	368.7

Net Changes in Boiler Fuel Fired

Fuel	#/hr	BTU/#	MMBTU/hr	MMSCFD	BTU/ft ³	BPSD
Crude Phenol	-14213	13070	-185.8			-920
Tar Oil	-47620	17000	-809.5			-3182
Fuel Gas	2440	18853	46.0	0.9	1228	
Naphtha	5768	20040	115.6			574
Export Steam	5280	1000	5.3			
Fuel Oil to Boiler	46004	18000	828.4			3217
Total	-2321		0.0	0.9		-201
Fuel Oil to Process Heaters	622	18000	11.2			45

Net Changes in SNS Production	ECV SNS MMSCFD	FSA/Purge Gas #mol/SL
SNS equivalent of Syn Gas to FSA	12.74	90591
SNS Credit for FSA Purge	8.40	41360
SNS Credit for HDS purge gas	0.12	506
Total SNS Production Loss	4.81	

Water Balance Hydrotreater

Component	H ₂ O	H ₂ S	NH ₃	NH ₄ HS	NH ₄ OH	Total
Reaction Gases	6839	218	602			7659
Reaction Solution	6317			327	1015	7659
Stripping Steam	1856					1856
Scattered Water	6826					6826
HDT Sour Water	14995			327	1015	16340

Water Balance Hydrocracker

Component	H ₂ O	H ₂ S	NH ₃	NH ₄ HS	NH ₄ OH	Total
Reaction Gases		0.5	0.5			1.0
Reaction Solution				0.8	0.5	1.3
Stripping Steam	556.9					556.9
HCR Sour Water	556.9			0.8	0.5	558.2

Total Sour Water

Component	H ₂ O	H ₂ S	NH ₃	NH ₄ HS	NH ₄ OH	Total
Total Sour Water	15556			328	1015	16898

APPENDIX B

AMOCO/DOE -

GREAT PLAINS GASIFICATION PLANT

JET FUEL FROM COAL DERIVED LIQUIDS

PROCESS DESIGN DESCRIPTION

CASE 3

MAXIMUM JP-8 PRODUCTION

SUBTASK 1.2

PRELIMINARY

LCI PROJECT 5571
DATE - DEC. 2, 1987

1.0 CASE DESCRIPTION

1.1 Overall Process Description

The purpose of this case is to maximize the production of type JP-8 aviation turbine fuel from Great Plains liquid by products. Figure 1 presents a block diagram for the process and referring to Figure 1 the flow is as follows:

- . Tar Oil byproduct stream (47620 #/hr, 3182 BPSD) is charged to the hydrotreater (Area 100).
- . The hydrotreater is a 3 stage expanded bed type process which removes 99% + of the sulfur, nitrogen, and oxygen compounds and begins the conversion of 550°F+ material. The hydrotreater adds a large quantity of hydrogen to the feed (4075 SCF/bbl) which results in a high heat of reaction. An expanded bed type reactor was chosen to both control and utilize the heat of reaction. Three stages were used to both control the temperature rise as well as to obtain the high efficiency associated with staging a back-mixed reactor.
- . The hydrotreater produces 6 streams:
 - High pressure purge gas (approximately 90% hydrogen) which is sent to the Rectisol Unit in the SNG plant for recovery of the H₂ and CH₄.
 - Low pressure fuel gas (75 psig) which is sent to the main boiler in the SNG plant.
 - Unstabilized naphtha which is sent to the combined naphtha stabilizer in the hydrocracker (area 200). After stabilization, to control vapor pressure, the naphtha is sent to the main boiler in the SNG plant.
 - JP-8 turbine fuel which is combined with JP-8 produced in the hydrocracker (area 200) and sent to storage.
 - 550°F+ unconverted bottoms product which is sent to the hydrocracker (area 200).
 - Wastewater containing, NH₄OH and NH₄HS which is sent to the PHOSAM unit in the SNG plant for recovery of the H₂S and NH₃.

- Approximately 950 #/day of spent catalyst which is shipped to a catalyst reclaimer in the same drums that the catalyst is received in.

The 550°F+ unconverted stream from the expanded bed hydrotreater (area 100) is charged to the fixed bed hydrocracker (area 200). The hydrocracker converts this material to naphtha and JP-8 turbine fuel. For this service a 5 stage unit was chosen with 65% conversion per pass. This unit also includes a naphtha stabilizer which stabilizes both the naphtha produced in the hydrotreater and hydrocracker.

The hydrocracker produces 4 streams in addition to JP-8

- High pressure purge gas (approximately 90% hydrogen) which is sent to the Rectisol Unit of the SNG plant for recovery of the H_2 and CH_4 .
- Low pressure fuel gas (75 psig) which is sent to the main boiler in the SNG plant.
- Stabilized naphtha which is sent to the main boiler in the SNG plant.
- A small sour water stream which is sent to the PHOSAM unit in the SNG plant or alternatively used as part of the injection water to the hydrotreating plant.

Hydrogen make-up for both the Hydrotreater and the Hydrocracker is supplied from a PSA Hydrogen Unit. High pressure (355 psig) synthesis gas from the Rectisol Unit (which contains about 63% hydrogen) is charged to the PSA unit which recovers 86% of the contained hydrogen as a high pressure 99.99% purity hydrogen gas product. The remaining purge gas is available at a low pressure (5 psig) which has a fuel value of about 565 BTU/ft³. This H_2 , CO & CH_4 rich gas is recompressed into the methanation unit of the SNG plant.

1.2 Overall Material Balance

The overall material balance is presented in Table 1.1 which presents overall material balances for the major process units. Detailed material balances for each unit can be found in appendixes A&B. The balance was computed on the basis that the fuel value of the feed will be replaced by fuel gas and naphtha produced in the process and the difference made up by the purchase of #6 Fuel Oil.

The overall balance is as follows:

Feeds

3182 BPSD of Tar Oil
1978 BPSD of #6 Fuel Oil
11.07 MMSCFD equivalent SNG product loss due to the syn gas feed
to the PSA unit.

Products

2490 BPSD of JP-8 turbine fuel
7.37 MMSCFD equivalent SNG product credit due to HDT, HDC & PSA
purge gas reinjection into SNG plant.

1.3 Overall Utility Balance

The overall utility consumption of the complex is as follows:

#6 Fuel Oil	1978 BPSD
SNG Equivalent	
of Syn Gas & Purge Gas	3.7 MM SCFD
Power	5450 kW
Cooling Water	2040 GPM (30°F rise)
Process Water	20.5 GPM

In addition the process exports 6945 #/hr of 100 psig saturated steam which was credited against boiler requirements.

Figure 1: Case 3 - Maximum JP-8 Production

Table 1.1: Great Plains Case 2: Maximum JP8 Production

Comp.	Wt %	Grav	#/hr	#Mole/hr	BPBD
Tar Oil Feed=====	47620		#/hr	3182	BPBD
JP-8 Product=====	24980		#/hr	2490	BPBD
SNG Product Loss=====	6275		#/hr	3.7	MMBtu/D
Fuel Oil Makeup=====	27386		#/hr	1978	BPBD

Expanded Bed Hydrocracker

Comp.	Wt %	Grav	#/hr	#Mole/hr	BPBD
Feeds					
HC	6.14		2925	1450.9	
Oil	100.00	1.0268	47620		3182
Total	106.14		50545		
Products					
Purge Gas	0.0		41	14.9	
Fuel Gas	1.87		891	43.9	
Naptha	10.17	0.7606	9127		823
JP-8	50.29	0.8720	27950		1978
SSO+BP+	24.4	0.9697	11660		825
H2S in SW	8.73		4159	271.1	
H2O in SW	0.47		201	4.0	
NH3 in SW	1.06		505	79.7	
Total	106.14		50545		3182

Fixed Bed Hydrocracker

Comp.	Wt %	Grav	#/hr	#Mole/hr	BPBD
Feeds					
HC	4.32		504	251.0	
SSO+BP+	100.00	0.9697	11660		825
Total	104.32		12164		
Products					
Purge Gas	2.88		336	113.5	
Fuel Gas	2.12		247	13.7	
Naptha	48.46	0.7148	5650		542
JP-8	50.86	0.7900	5930		515
H2S in SW	0.003		0.4	0.01	
NH3 in SW	0.003		0.4	0.02	
Total	104.32		12164		1057

Naptha Stabilizer

Comp.	Wt %	Grav	#/hr	#Mole/hr	BPBD
HDT Nap	61.76	0.7606	9127		823
HCB Nap	38.24	0.7148	5650		542
Stab Nap	97.75	0.7346	14445		1749
Fuel Gas	2.25		332	7.8	

PSA Hydrogen Recovery Unit (86% Recovery)

Component	H ₂	CO	CO ₂	CH ₄	C ₂ H ₆	N ₂ +Ar	Total
Mol %							
Feed Gas	116.28	34.26	2.72	29.84	0.52	0.35	184.07
Prod. H ₂	100.00	0.01					100.01
Purge Gas	16.28	34.25	2.72	29.84	0.52	0.35	84.02
Wt %							
Feed Gas	116.28	475.95	59.44	237.46	8.67	5.55	900.31
Prod. H ₂	100.00	0.12	0.00	0.00	0.00	0.00	100.12
Purge Gas	16.28	475.83	59.44	237.46	8.63	5.55	892.19
#(mol)/hr							
Feed Gas	1977.8	582.7	46.3	507.5	9.9	6.0	7130.2
Prod. H ₂	1700.9	0.2	0.0	0.0	0.0	0.0	1701.1
Purge Gas	276.9	582.6	46.3	507.5	9.9	6.0	1429.1
#/hr							
Feed Gas	3587	16320	2038	8143	296	190	70124
Prod. H ₂	3429	4	0	0	0	0	3431
Purge Gas	558	16316	2038	8143	296	190	70124

Fuel Gas Generated in Hydrotreating and Hydrocracking

Component	#/hr	#Mol/hr	MMBtu/hr
HDTB FG Produced	841	43.9	16.0
HCB FG Produced	142	13.7	4.4
Stab FG Produced	730	7.8	2.0
Total Fuel Gas	1470	65.4	26.5

Purge Gas Generated in PSA Hydrogen Unit

Component	#/hr	#Mol/hr	BTU/ft ³	MMBtu/hr
H ₂	558	276.9	324	34.0
CO	16316	582.6	321	70.9
CO ₂	2038	46.3	0	0.0
CH ₄	8143	507.5	1010	194.3
C ₂	296	9.9	1769	6.6
N ₂ +Ar	190	6.0	0	0.0
Total	27541	1429.1	565	305.8

Net Charges to Boiler Fuel Fired

Fuel	#/hr	Btu/#	MMBtu/hr	MMBtu/D	Btu/ft ³	Btu/D
Tar Oil	47620	17000	809.5			7182
Fuel Gas	1470	19000	28.5	0.6	1068	
Naphtna	14445	20040	289.5			1745
Export Steam	6745	1000	6.9			
Fuel Oil to Boiler	27536	18000	495.7			1750
Total	22777		0.0	0.6		11

Fuel Oil to Process Heaters	350	18000	6.3			28
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Net Charges to SNG Production	MMBtu/D	PSA Fuel Gas
PSA equivalent of SNG Gas to PSA	11.12	75124
SNG Credit for PSA Fuel Gas	6.9	11.12
SNG Credit for PSA Fuel Gas	0.47	3091
Total SNG Production Loss	3.65	

Water Balance Hydrocracker

Component	H ₂ O	H ₂ S	NH ₃	NH ₄ HS	NH ₄ OH	Total
Reaction Gases	4156	105	5.8			4865
Reaction Solution	1733			308	519	4865
Stripping Steam	1228					1228
Distilled Water	9281					9281
HRT Sour Water	14235			308	829	15601

Water Balance Hydrocracker

Component	H ₂ O	H ₂ S	NH ₃	NH ₄ HS	NH ₄ OH	Total
Reaction Gases		0.4	0.4			0.7
Reaction Solution				0.5	0.4	0.9
Stripping Steam	225.1					225.1
HCR Sour Water	225.1			0.5	0.4	226.0

Total Sour Water

Component	H ₂ O	H ₂ S	NH ₃	NH ₄ HS	NH ₄ OH	Total
Total Sour Water	14464			308	829	15601

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