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BASELINE DESIGN/ECONOMICS FOR ADVANCED FISCHER-TROPSCH TECHNOLOGY. QUARTERLY REPORT, JANUARY--MARCH 1993

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U.S. Department of Energy Pittsburgh Energy Technology Center

Baseline Design/Economics for Advanced Fischer-Tropsch Technology

Contract No. DE-AC22-91 PC90027

Quarterly Report

January - March 1993

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Section 1 Introduction and Summary

This report is Bechtel's sixth quarterly technical progress report and covers the period of January through March, 1993.

1.1 INTRODUCTION

Bechtel, with Amoco as the main subcontractor, initiated a study on September 26, 1991, for the U.S. Department of Energy's (DOE's) Pittsburgh Energy Technology Center (PETC) to develop a computer model and baseline design for advanced Fischer-Tropsch (F-T) technology. This 24-month study, with an approved budget of \$2.3 million, is being performed under DOE Contract Number DE-AC22-91PC90027.

The objectives of the study are to:

- Develop a baseline design and two alternative designs for indirect liquefaction using advanced F-T technology. The baseline design uses Illinois No. 6 Eastern Coal and conventional refining. There is an alternative refining case using ZSM-5 treatment of the vapor stream from the slurry F-T reactor and an alternative coal case using Western coal from the Powder River Basin.
- o Prepare the capital and operating costs for the baseline design and the alternatives. Individual plant costs for the alternative cases will be prorated on capacity, wherever possible, from the baseline case.
- o Develop a process flowsheet simulation (PFS) model.

The baseline design, the economic analysis and computer model will be major research planning tools that PETC will use to plan, guide and evaluate its ongoing and future research and commercialization programs relating to indirect coal liquefaction for the manufacture of synthetic liquid fuels from coal.

The study has been divided into seven major tasks:

- o Task 1: Establish the baseline design and alternatives.
- o Task 2: Evaluate baseline and alternative economics.
- o Task 3: Develop engineering design criteria.
- o Task 4: Develop a process flowsheet simulation (PFS) model.
- o Task 5: Perform sensitivity studies using the PFS model.

- o Task 6: Document the PFS model and develop a DOE training session on its use.
- o Task 7: Perform project management, technical coordination and other miscellaneous support functions.

1.2 SUMMARY

During the reporting period, work progressed on Tasks 1, 4 and 7. This report covers work done during the period and consists of four sections:

- o Introduction and Summary.
- o Task 1 Baseline Design and Alternatives.
- o Task 4 Process Flowsheet Simulation (PFS) Model.
- o Project Management and Staffing Report.

Completed work on Task 1, during the period of this report, consisted mainly of finalizing the Baseline Case process design of Area 200, F-T Synthesis, and Area 300, Product Upgrading and Refining. Process design for Area 100, Syngas Production, was reported in the Third and Fourth Quarterly. For each plant within the areas 200 and 300, its design basis, criteria and considerations, PFD and process description, and complete material balance are now reported

Under Task 4, preliminary Baseline Case simulation model for the F-T reactor loop has been completed and now reported. Individual plant models were also developed for all the units in Area 300, Product Upgrading and Refining section. A complete model, tying all the above developments with the Area 100 model that was reported in the last quarterly, is currently under development.

Under Task 7, cost and schedule control was the primary activity. A technical progress meeting was planned, project progress reviewed and inputs implemented.

Section 2 Task 1 - Baseline Design and Alternatives

Work progressed during this quarter mainly with the Baseline design case. Process designs for both Area 200, F-T Synthesis, and Area 300, Product Upgrading and Refining, were finalized. Design information for Area 100 was reported in the Third and Fourth Quarterly Reports, including the following plants in the Syngas Production Section (the number of on-stream trains is shown for each plant):

Plant 101	Coal Receiving and Storage (1 train).
Plant 102	Coal Drying and Grinding (5 trains).
Plant 103	Shell Coal Gasification (8 trains).
Plant 104	COS/HCN Hydrolysis (8 trains).
Plant 105	Sour Water Stripping (1 train).
Plant 106	Acid Gas Removal (4 trains).
Plant 107	Sulfur Plant (Claus/TGT) (2 trains).
Plant 108	Sulfur Polishing (8 trains).
Plant 109	Syngas Wet Scrubbing (8 trains).
Plant 110	Air Separation (8 trains).

2.1 BASELINE DESIGN CASE - AREA 200

2.1.1 Plant 201 - Fischer-Tropsch Synthesis

The principle function of this plant is to convert syngas from Area 100 into hydrocarbon products using slurry phase Fischer-Tropsch reactors. Since the syngas conversion per pass is 81.6%, Plant 201 is part of an overall recycle synthesis loop which is called Area 200.

Design Basis and Considerations

A total of 24 operating reactors are required to process the syngas from 20,000 TPD of Illinois No. 6 coal. A total of 25 reactors are provided, with 24 in operation and 1 spare. A total of 8 trains are needed down stream of the F-T reactors to process the F-T reaction products. This section of the plant is not spared. The reactors are

manifolded so that shutting down a reactor affects all downstream trains equally, which minimizes turndown. The number of operating trains required for different areas of Plant 201 is indicated on the respective PFD's.

Mobil's pilot plant data were utilized to develop the design correlations for predicting wax yield and overall product distribution (including oxygenates) versus reactor temperature. A detailed description of this analysis was presented in January-March 1992 Quarterly report. An analysis was made of the economics of running to various wax yields. The final baseline design condition selected consists of an F-T reactor operating temperature of 487.6 °F, an operating pressure of 289 psig and a wax yield of 50 wt%.

Reactor sizing is based on the Bechtel reactor design model described in the final report under DOE Contract DE-AC22-89PC89867, as modified for this study. The primary modification was that the catalyst activity expression was obtained by applying this model to the Mobil pilot plant data. Reactor sizing calculations, using the Bechtel model, were used to set 70.5 % hydrogen conversion as the design basis. With the design H2/CO inlet ratio (0.361 in the Area 100 syngas and 0.460 at the reactor inlet) and water vapor addition rate, the yield model shows that CO conversion is 86.8 % and overall H2 + CO conversion is 81.6 mole%. A total of 5405 lbmol/hr of water vapor is added in a saturator ahead of the reactor to bring the water concentration in the reactor inlet gas to 6.6%. This water compensates for the low H2/CO ratio by promoting additional H2 formation in the reactor via the water gas shift reaction.

Catalyst replacement has been specified at 0.5 % per day of total catalyst inventory. The catalyst concentration in the slurry phase has been specified at 22.5 wt%, and the inlet gas velocity has been set at 10 cm/s, since these are the most severe conditions demonstrated in actual pilot plant operations to date. The heat of reaction is removed by medium pressure steam generation in bayonet tubes suspended from a double tubesheet inside the reactor.

Process Description (PFD 201-B-01.02.03)

The process flow diagrams for Plant 201, F-T Synthesis, are shown in PFD 201-B-01 through PFD 201-B-03.

The syngas from Plant 108, Sulfur Polishing is humidified in 201C-1 (only one required for the whole facility) using a spray of boiler feed water and is mixed with the recycle gas stream from the autothermal reformers (Plant 206). The combined gas stream enters the F-T reactor at 362 °F through a cylindrical gas distributor. In the F-T reactor, the syngas bubbles upward through the catalyst/wax slurry, dissolves in

the slurry phase and is converted into hydrocarbon products at the catalyst interface. The slurry consists of a 22.5 wt% mixture of catalyst suspended in the nonvaporizable portion of the liquid product (i.e. the wax).

As shown in the process flow diagram PFD 201-B-01, the catalyst/liquid wax stream is withdrawn from the F-T reactor at 488 °F and 289 psig and passed through a hydroclone (201T-2) to produce an overflow stream containing about 12 wt% catalyst and an underflow stream of about 45 wt% catalyst. Roughly 65 % of the catalyst is recovered in the underflow and is pumped back to the reactor. The design is based on an assumed average catalyst particle size of 34 microns.

The overflow from the top of the hydroclone is passed through a valve to reduce pressure from 289 to 70 psig (PFD 201-B-02) and sent to a product separator (201C-8). The pressure reduction causes dissolved gases to separate from the liquid product stream. The vapors from 201C-8 are cooled to 100 °F to recover additional liquid and are sent to fuel. The liquid is sent to the F-T liquid wax intermediate hold tank, 201C-10, which serves as the feed drum for the wax clarifying, catalyst recovery filters, 201T-4A,B. These are enclosed washing type cake filters, using naphtha from downstream processing to recover the wax left in the catalyst cake. The wax is recovered from the wash by distillation and combined with the clear wax from the filter. The clear wax stream from Plant 201 then is sent to the hydrocarbons recovery plant, Plant 204.

A heated, agitated holding tank is provided for slurry storage during reactor shutdown. This slurry can be returned to the reactor after repairs are made. Occasionally there may be a need to discard a bad batch of catalyst or to remove fines. This is done via the catalyst filters, 201T-4, and spare capacity is provided for this purpose.

The catalyst from 201T-4 is stripped of naphtha in a heated screw conveyor and most of it is recycled back to the reactor slurry feed drum. About 20 tons per day is removed to disposal to counteract catalyst makeup and maintain catalyst inventory in the reactors. The recovered naphtha is recycled. The design of the F-T catalyst separation and recovery system is not very rigorous. Design basis for an effective F-T catalyst separation method is not readily available. The selected scheme represents only a best engineering estimate, based on our current knowledge of the catalyst system, its characteristic and commercial separation equipment available.

As shown in PFD 201-B-01, the overhead vapor stream from F-T reactor is passed through a cyclone separator 201T-1 to disengage any liquid carryover. The vapor stream at 488 °F and 289 psig is cooled to 100 °F in heat exchanger 108E-2, air cooler 201E-3 and water cooler 201E-2 (PFD 201-B-02). The cooled stream is sent to a three

phase separator 201C-6, wherein the aqueous water stream, the liquid hydrocarbons stream and the vapor stream are separated.

The aqueous water stream from 201C-6 is sent to the waste water treatment facility. The liquid hydrocarbons stream is sent to Plant 204 along with the wax from the catalyst filters. The overhead vapor stream from 201C-6 is passed through a vapor phase oxygenates water wash column, 201C-7, to separate vapor phase oxygenates from the unconverted syngas. The waste water stream from the bottom of column 201C-7 is also sent to the treatment facility. The unconverted syngas stream, after oxygenates removal, is sent to the CO₂ recovery plant, Plant 202.

It is estimated that 20 TPD of makeup catalyst is required to maintain the catalyst inventory level in the F-T reactors. Process flow diagram PFD-201-B-03 shows the batchwise catalyst pretreatment facility which provides a continuous supply of activated, makeup catalyst. Clear wax from storage is preheated to 450 °F in heat exchanger 201E-6 using 600 PSIG saturated steam. The preheated wax is used to fill catalyst pretreater, 201C-11, and dry fresh catalyst from hopper 201T-6 is added up to the design concentration of 22.5 % by weight.

The system is filled with syngas and catalyst activation is carried out batchwise in 201C-11 by circulating preheated syngas at 487 °F and 195 PSIG. The activation reactions are the reduction and carbiding of the catalyst but some hydrocarbon product may be produced as well. The activation gas is circulated through coolers and a separator for hydrocarbon and water removal. Then it is compressed and reheated to activation temperature. Composition adjustments may be made by the addition of syngas, hydrogen and/or nitrogen.

The activated catalyst/wax slurry is withdrawn from the bottom and sent to the slurry storage tank, 201C-12, where it is maintained at 487.6 °F using a hot oil circulation loop before it is pumped semi-continuously to the F-T reactors. A single train of the catalyst pretreatment plant, 201-B-03, is required for all reactors. It is operated for only 8 hours/day.

Technology/Licensor Selection

The design of Plant 201 is based on in-house correlations. Hydrocione Information was obtained from Dorr-Oliver.

Material Balance

The material balance for Plant 201 is shown in Table 2-1. In performing F-T reactor material balance, it is assumed that all of the vapor phase oxygenates remain in the vapor stream, all of the water phase oxygenates remain in the aqueous water stream

(201.6) and the hydrocarbon phase oxygenates are distributed between the wax (201.5) and liquid hydrocarbons stream (201.3).

2.1.2 Plant 202 - Carbon Dioxide Removal

Design Basis and Considerations

CO₂ is the primary byproduct in the F-T reactor when operated at low H₂/CO ratios with a catalyst active for the water gas shift reaction. It must be removed from the F-T recycle loop recycle gas before the gas is returned to the reactor and, the sooner this is done, the better, since this reduces the size of the downstream equipment. The general process requirements and preferences for the CO₂ removal unit are as follows:

- (1) The CO₂ removal system preferably should operate at loop pressure before the gas is recompressed in the recycle compressor (approximately 269 psig);
- (2) The CO₂ stream preferably should be produced at elevated pressure and has to be free of hydrocarbons and inert gases (such as nitrogen) so it can be used in the gasifier coal feed system (Plant 102) without further compression or purification;
- (3) If vented to the atmosphere without additional treatment, the CO₂ stream must be low in contaminants;
- (4) The recycle gas after CO₂ removal must be sufficiently low in CO₂ (e.g. less than 400 ppm) so that it will not freeze out in the cryogenic section of the hydrocarbon recovery unit in the gas plant (Plant 204) and plug up the heat exchangers and other equipment;
- (5) Low cost and low energy consumption are preferred.

Chemical solvents involving amines are favored for this service because of lower capital investment cost and reasonable energy requirements compared to other technologies. Furthermore, inhibited MDEA (a tertiary amine) or glycol amines are preferred over high concentration MEA (a primary amine) with corrosion inhibitors because there is less of a disposal problem of the spent solutions. Any of these amines will produce a recycle gas with a CO₂ concentration well below the 400 ppm specification. More detailed analysis of alternative CO₂ removal technologies was performed in the Tradeoff Studies, and the results were documented in the Quarterly Report for April-June 1992 for this project.

Technology/Licensor Selection

There are several proprietary amine solvents such as Gas/Spec (Dow Chemical), UCARSOL (Union Carbide), Amine Guard (UOP), Flexsorb (Exxon), etc. which

contain high concentrations of either MDEA or glycol amines plus proprietary additives. There is not much difference between these processes from a heat requirement or cost standpoint. The major difference is in the types of the corrosion protection schemes.

Dow's Gas/Spec process, which uses a 50 wt% MDEA solution plus proprietary additives, is selected as a representative process for the process design.

Process Description (PFD 202-B-01)

The process flow diagram for the CO₂ removal plant (Plant 202) is shown in PFD 202-B-01. This plant is configured similarly to the Acid Gas Removal Plant (Plant 106) which also is an amine unit. Eight (8) parallel Plant 202 trains are required. The vapors from the F-T high pressure separator (Plant 201 F-T Synthesis) and the off-gas from the deethanizer overhead (Plant 204 F-T Gas Plant) are combined in the feed gas KO drum 202D-1 and sent to the amine adsorber (202C-1) for CO₂ removal.

To ensure an amine-free vapor product, the adsorber overhead vapor is waterwashed in scrubber 202C-3, and the liquid is returned to the rich-amine knock-out drum, 202-D2. The rich-amine solution from the bottom of adsorber is flashed in 202-D2, and heated by exchange with the lean-amine solution before being sent to one of the two Amine Regenerators, 202C-2A or B.

Because of the high reboiler duty caused by the high CO₂ removal rate, two (2) amine regenerators are required for each amine adsorber. Each regenerator is in turn serviced by four (4) reboilers. The regenerated lean-amine solution from these two regenerators is combined and pumped to a common amine storage tank 202D-3. The lean-amine then is pumped from this tank, cooled and sent back to the adsorber. A portion, approximately 10%, of the cooled lean-amine solution is filtered and returned to the storage tank.

A portion of the CO₂ gas from the regenerator overhead separators (202C4A and B) is sent to Plant 102 for use as carrier gas in the gasifier lock hoppers. Excess CO₂ is vented to atmosphere.

Material Balance

The material balance for Plant 201 is shown in Table 2-2.

2.1.3 Plant 203 - Recycle Gas Compression and Dehydration

Recycle gas from Plant 202 (CO₂ Removal) is sent to this plant to increase the recycle loop pressure and remove the moisture in order to satisfy the requirements of recycle loop hydraulics and downstream hydrocarbon recovery at low temperatures. Four (4) parallel trains are provided, and there is no spare train.

Design Basis and Considerations

Recycle Gas Compression:

Four (4) parallel compression trains are provided to help maintain system startup and turndown capabilities and to tie in with the rest of the recycle loop. The compressors raise the pressure of the recycle gas from 250 to 425 psig. An aftercooler condenses the water which is returned to the humidifier in Plant 201.

Dehydration:

A molecular size type dryer is used to reduce the moisture content to approximately 0.1 ppm to prevent hydrate formation in the downstream cryogenic hydrocarbon recovery unit where the temperature could be as low as -145°F.

Each dehydration train has two (2) parallel adsorber vessels. While one is on the adsorption cycle, the other is on regeneration cycle. Each cycle lasts eight (8) hours. The regeneration cycle is further broken down as follows:

Purging	5.5 hr
Cooling	2.5 hr.

A portion of the fuel gas generated at the Hydrogen Recovery Plant (Plant 205) will be used for adsorber regeneration before being sent to the fuel gas header system. The pressure of this gas is adequate without compression.

Process Description (PFD 203-B-01)

The process flow diagram of the Compression and Dehydration process is shown in PFD 203-B-01.

The recycle gas from the CO₂ removal plant, Plant 202, is passed through a flash drum 203C-1 in which some of the hydrocarbons condense and are sent to Plant 204. The overhead gas stream from 203C-1 is sent to compressor 203K-1 to boost the pressure to 425 psig. It is then cooled from the compressor outlet temperature of 195

°F to 100 °F in water cooler 203E-1 and passed through a KO drum 203C-2 to condense water, which is returned to Plant 201.

The gas stream enters the dehydration section containing the two adsorber, 203C-3A and B. One vessel acts as the adsorber while the second vessel is being regenerated. A fuel gas stream of 4920 moles per hour from Plant 205 is used as the regenerating medium.

The unconverted syngas stream from the dehydration step is sent to Plant 204.

Technology/Vendor Selection

UOP's molecular sieve process serves as the basis for dehydration unit design.

Material Balance

The material balance for Plant 201 is shown in Table 2-3.

2.1.4 Plant 204 - Hydrocarbon Recovery

This plant :

- (1) Recovers the C3/C4 hydrocarbons and pentene from the recycle gas as feed for the alkylation unit,
- (2) Fractionates the heavier hydrocarbon liquids into naphtha, distillate, and wax for upgrading at Plants 303, 302 and 301, respectively.
- (3) Provides a lean recycle gas feed for Hydrogen Recovery Plant (Plant 205) which subsequently goes to the Autothermal Reformer Plant (Plant 206) and then to the F-T Synthesis (Plant 201)

Design Basis and Considerations

Approximately 95% of the Fischer-Tropsch C₃/C₄ hydrocarbons which are present in the recycle gas are recovered in Plant 204 by condensation at -140 °F followed by deethanization. An ethylene/propane cascade refrigeration system is employed. A depentenizing step also is included to recover C5 olefins for subsequent alkylation. The C5 saturates are included in the product naphtha which goes to hydrotreating (Plant 302) and eventually end up in the C5/C6 isomerization plant (Plant 306) feed.

Portions of oxygenates present in the hydrocarbon phase, principally methanol, will probably end up in the alkylation feed. A water wash column is provided to

remove the oxygenates since they tend to increase the sulfuric acid usage during alkylation.

Plant 204 also includes a liquid product fractionator. The cut points for the liquids are listed below:

Naphtha	C5 saturates - 350 °F
Distillate	350 °F - 650 °F
Wax	650 °F +

A total of 4 trains are provided.

Process Description (PFD 204-B-01.02.03)

Process flow diagrams PFD 204-B-01 through PFD 204-B-03 show the configuration of the hydrocarbons recovery plant.

As shown in PFD 204-B-01, the unconverted syngas stream leaving the Compression and Dehydration Plant (Plant 203) is divided into two streams which are both cooled to -100 °F against -140 °F condensed vapor and liquid, respectively, in heat exchangers 204E-5 and 204E-6. The two streams are recombined, further cooled to -140 °F and partially condensed in heat exchanger 204E-4 using -150 °F ethylene refrigerant. The ethylene is in turn condensed by propylene refrigeration at -37 °F in a standard cascade cycle.

Vapor and liquid fractions are recovered at -140 °F in separator 204C-3. Approximately 95% of the C3/C4 hydrocarbons present in the recycle syngas are recovered. Both vapor and liquid streams are reheated to approximately 85 °F in heat exchangers 204E-5 and 204E-6. The vapor stream is sent to Plant 205, Hydrogen Recovery. The liquid stream is sent to the deethanizer, (204C-4 on PFD 204-B-02).

Process flow diagram PFD 204-B-02 shows the deethanizer tower, depentenizer tower, and the water wash column. Liquid hydrocarbons from Plants 201 and 203 are combined with the liquid from 204E-6 and enter the deethanizer tower on the fifth tray. The deethanizer tower contains 19 trays. The overhead vapor from the deethanizer tower (H2, CO2, N2, C1 and C2's) is partially condensed at -12 °F against propylene refrigerant in exchanger 204E-7 and sent to reflux accumulator drum 204C-5 where gases are separated from the hydrocarbon liquid which is refluxed back to the tower. A water draw is provided on tray 3. The net overhead vapor stream is the lean recycle gas and it is sent to Plant 202, CO2 Removal. Reboiler 204E-8 at the bottom of the deethanizer tower is supplied with 365 psig saturated steam. The bottoms stream flows to the depentenizer, 204C-7.

In the depentenizer tower, propane through pentenes are taken overhead. The depentenizer tower contains 83 trays. The overhead vapor stream is condensed at 100 °F against cooling water in exchanger 204E-9 and sent to the reflux accumulator, 204C-8. A part of the liquid hydrocarbon is refluxed back to the tower and the remainder is withdrawn as the overhead product which flows to the water wash column, 204C-9. The bottoms flow to the product fractionator, 204C-10 (on PFD 204-B-03). The depentenizer is reboiled with high pressure steam.

Methanol and other light oxygenates in the depentenizer overhead are removed by a water wash in the oxygenates wash column, 204C-9. The water wash column is a packed tower containing 1" metal pall rings. The bottoms water stream containing dissolved light oxygenates is sent to the waste water treatment facility. The clean C3- $C5^{=}$ overhead stream goes to the alkylation plant in Area 300.

As shown in PFD 204-B-03, the depentenizer bottoms stream is mixed with the wax stream from Plant 201, F-T Synthesis. The combined stream is reduced in pressure from 140 psig to 27 psig and flashed in separator 204C-10 to separate the vapor and liquid. The liquid stream from the bottom of separator 204C-10 is preheated from 437 °F to 553 °F, (against tower bottoms) in heat exchanger 204E-11 and further heated to 680 °F in direct fired heater 204F-1 before entering the product fractionator tower on tray 19. The vapor is fed on tray 17.

The function of the fractionator tower is to separate liquid hydrocarbons into naphtha, distillate and wax products which are sent to Area 300 for final upgrading. The fractionator tower contains 21 trays. The fractionator overhead vapor stream tower is cooled from 248 °F to 100 °F in air cooler 204E-12 and water cooler 204E-13 before entering the three phase accumulator, 204C-12. In the accumulator 204C-12, a small amount of vapor is separated and sent to flare. The condensed water stream produced as a result of utilizing live stripping steam, is sent to the waste water treatment facility. A portion of the liquid hydrocarbon stream is refluxed back to the tower, and the remainder is withdrawn as the net naphtha stream.

A 5 tray side stripper stabilizes the liquid drawn from tray 7 of the fractionator tower to provide a distillate product stream. Saturated steam at 50 psig is used as the stripping medium.

The bottom wax stream from the product fractionator is cooled from 628 °F to 470 °F in heat exchanger 204E-11 before being sent to the wax hydrocracker, Plant 301.

Technology/Vendor Selection

Open art technology is utilized.

Material Balance

The material balance for Plant 201 is shown in Table 2-4.

2.1.5 Plant 205 - Hydrogen Recovery

This plant provides the high purity H₂ required for the upgrading section (Area 300). The feeds are recycle gas from Plant 204 and hydrogen-rich offgas from the Catalytic Reformer, Plant 304.

Design Basis and Considerations

A total of four (4) parallel trains are required to provide 27.63 MMSCFD of high purity H2 (99.99 mol%) utilizing the polybed pressure swing adsorption process. Each train utilizes ten PSA adsorber vessels, packed with molecular sieves, which are cycled in sequence at from 380 psig to 100 psig.

Four (4) parallel trains are used to be compatible with the other plants in the recycle loop.

Process Description (PFD 205-B-01)

The process flow diagram of the hydrogen recovery PSA unit is shown in PFD 205-B-01.

A slipstream of recycle gas from Plant 204, Hydrocarbons Recovery, is combined with the off-gas stream from the Catalytic Reformer, Plant 304. The combined gas stream flows through a K.O. drum, enters the feed valve, and flows upward through the adsorbër vessel. As the gas flows upward through the adsorber the impurities present in the gas are selectively adsorbed. To maximize hydrogen recovery an adsorber is switched from an adsorption position when the impurities front has reached a predetermined level in the adsorber. When an adsorber which has just been regenerated has reached adsorption pressure, it is switched to the adsorption step and the first adsorber begins its regeneration sequence.

Several cocurrent blowdown steps are performed to regenerate a bed. Initially, the pressure in the adsorber is reduced to desorb hydrogen. Pure hydrogen leaving at the top of the adsorber is internally used in the PSA unit to repressurize and purge other adsorbers. The so-called co-current or upward pressurization step is terminated when the impurities front reaches a second predetermined position in the bed. At this point, little hydrogen is left in the adsorber and the reduced pressure has started desorption or impurities. The flow in the adsorber is then reversed, and

the adsorber is depressurized downward to off-gas pressure. In actuality, the regeneration process involves several pressure equalization and depressurization steps which are performed automatically.

The product stream from the PSA unit is sent to Area 300, Upgrading and Refining. The reject stream is combined with the recycle loop purge stream and sent to Plant 203 to be used as regeneration gas in the dryer and to supply the fuel gas requirements for the facility. The main recycle gas stream flows on to Plant 206, Autothermal Reforming.

Technology/Vendor Selection

Union Carbide's PSA polybed process is selected for this application. The unit is a standard ten-bed PSA system. A bank of ten vessels filled with adsorbent, valve assemblies with piping and instrumentation and a control panel are assembled on a skid.

Material Balance

The material balance for Plant 201 is shown in Table 2-5.

2.1.6 Plant 206 - Autothermal reformer

Design Basis and Considerations

The autothermal reformer is included in the recycle loop to:

- (1) Minimize the built-up of light ends by converting them to syngas. This will produce more F-T liquids and improve the overall economics.
- (2) Help modify the H2/CO ratio in the F-T feed stream to satisfy the target conversions of H2 and CO in the F-T reactors.
- (3) Provide operating flexibility such that an unexpected failure of the Gas Plant (Plant 204) does not cause the shutdown of the entire recycle loop. In this case the gas stream, containing unrecovered C3/C4 hydrocarbons, can be bypassed to Plant 206 for disposal. For this matter, excess plant fuel gas also can be sent to this plant to be converted to valuable F-T feedstock.

A reactor feed/effluent heat exchange system is incorporated in the design for reasons of efficiency. A waste heat boiler and feed charge heater system would cost about the same, but would be less energy efficient.

Technology/Vendor Selections

Autothermal Reaction System Both Lurgi Corporation of Germany and Haldor Topsoe, Inc. of Houston, TX are licensors of autothermal reforming technology. In the baseline design, Lurgi's technology is used because of their commercial experience at Sasol.

Autothermal Reforming Catalysts Lurgi would use catalyst supplied by vendors such as United Catalysts, Inc. Haldor Topsoe would provide their own catalyst.

Reactor Feed/Effluent Heat Exchangers

Due to the high temperature differentials (reactor effluent cooling from 1800°F to 500°F and reactor feed heating from 72°F to 1400°F), the heat exchanger metallurgy and internal mechanical design require special attention. A TEMA AFT shell-and-tube heat exchanger with four (4) shells in series and countercurrent flow would meet the thermal design criteria. However, the design of internals, such as the stress considerations for the tubesheet and shell, need first-of-its-kind calculations. While this high-temperature/high-pressure design principle has been demonstrated in ICI's Gas Heated Reformer and used in hydrogen and ammonia plant designs, heat exchanger vendors do not yet fabricate such equipment for standard heat exchange services.

In order to eliminate the tubesheet and the exposure of the shell inside wall to high temperatures, Struthers Wells Corporation of Warren, PA has proposed a feed superheater to replace the first two shell-and-tube heat exchangers which see the highest temperatures. This feed superheater would be internally lined with the refractory and would be similar to a superheater box using hot furnace flue gas to superheat other process gases or steam, except that this feed superheater box would be under pressure.

Process Description (PFD 206-B-01)

The process flow diagram of the autothermal reforming plant (Plant 206) is shown in PFD 206-B-01. The oxygen feed from the air separation plant (Plant 110) is heated to 500°F by high pressure steam in heat exchanger 206E-2. The warm oxygen is subsequently combined with the process steam before being sent to the mixing chamber located at the top of the autothermal reforming reactor, 206C-1. The preheated feed gas also is introduced to this mixer via separate nozzles. The mixing chamber and the reactor are proprietary designs of the licensors.

The normal autothermal reformer reactor outlet temperature is 1,800°F. The combined recycle gas from the hydrogen recovery plant (Plant 205) at a temperature

of approximately 72°F is heat exchanged with the autothermal reformer effluent to reach a feed preheat temperature of 1706°F. The heat exchange takes place in feed superheater 206E-1 and heat exchangers 206E-3A & B. As a result, the reactor effluent is cooled to 500°F before being sent to the F-T reactors in Plant 201. Preheat levels are maximized to minimize oxygen consumption. No steam is produced using this heat exchange arrangement.

Four (4) parallel reactor heat exchanger trains are provided for this service. This four train configuration is dictated by a combined consideration of turndown capability of the autothermal reformers and pressure drop limitations of the superheater and heat exchangers.

Material Balance

The material balance for Plant 201 is shown in Table 2-6.

2.2 BASELINE DESIGN CASE - AREA 300

Fischer-Tropsch synthesis produces a wide spectrum of hydrocarbon products which are not directly usable in their raw states. Upgrading is required to produce highquality transportation fuels. Area 300 of the Baseline Case uses conventional technologies to upgrade and refine the F-T products to high-quality fuels. It is designed to produce maximum amounts of high-octane gasoline and high-cetane diesel blending stocks. An alternate upgrading scheme also will be studied, as part of the overall project, at a later time.

The overall block-flow diagram for Area 300 is shown in Figure 2-1. Streams leaving the F-T Product Fractionator from Area 200, Plant 204, enter the various catalytic processing units as shown, together with the required hydrogen and purchased n-butane. Other products include C2- fuel gas and C3 LPG. No attempt was made to rigorously design all the processing units in Area 300. Detailed PFD's, therefore, are not given. However, rigorous material balances, along with detailed utility and capital investment requirements are developed in this study.

This section gives a brief description of each processing unit, its objective, and process selection criterion. Material balance for Area 300 is shown in Table 2-7.

2.2.1 PLANT 301 - WAX HYDROCRACKING

Objective: To catalytically crack the F-T wax product under a hydrogen environment to yield more desirable gasoline and diesel products.

Type: Single stage fixed-bed hydrocracker

Selection Rationale:

The process allows extensive cracking of the wax with minimum coke formation. It yields high quality diesel products.

Process Description:

A typical process flow diagram is shown in Figure 2-2. Fresh feed is combined with unconverted feed and hydrogen (both recycled and makeup), preheated in a furnace and then fed to the fixed-bed reactor(s). Reactor effluent is cooled and sent to a high pressure separator. Separator gas is compressed and recycled back along with the makeup hydrogen to combine with the fresh feed. The separator liquid is sent to a low pressure separator where the overhead gas goes directly to the Saturated Gas Plant. The liquid is routed to a series of separation towers for product fractionation. Unconverted feed from the fractionator bottom stream is recycled back and mixed with the fresh feed.

Product Streams:

Diesel (301.4) C7+ Gasoline (301.3) C5/C6 (301.2) C4- fuel gas (301.1)

Major Equipment/Features:

Reactor(s)

- 15,000 40,000 BPSD unit
- 2 in series, one train
- ~700 F/1100 Psig

Preheat furnace High and low pressure separator Hydrogen compressors Debutanizer tower Dehexanizer tower

Product fractionator

2.2.2 Plant 302 - Distillate Hydrotreating

Objective: To remove oxygen containing compounds and saturate olefins to produce a high-cetane diesel product.

Type: Fixed-bed hydrotreaters

Selection Rationale:

The process is desirable to meet final product quality.

Process Description:

A typical process flow diagram is shown in Figure 2-2. Distillate feed from Area 200, Plant 204, is heated via heat exchange with the reactor effluent, mixed with makeup and recycled hydrogen, and heated in a single-pass furnace. The hot mixture is charged into the fixed-bed hydrotreating reactor. Reactor effluent is cooled and sent to a high-pressure separator where the overhead separator gas is compressed and recycled back along with the makeup hydrogen to combine with the fresh incoming feed. Separator liquid is sent to a low-pressure separator where the gas goes directly to the saturated gas plant. The separator liquid is charged to a splitter tower in which additional light ends are removed from the diesel product to meet the product flash point specifications. The unit has an expected onstream factor of 96%.

Product Streams:

Diesel (302.2) Fuel gas (302.1)

Major Equipment/Features:

Reactor Feed/hydrogen furnace Feed/effluent exchanger High pressure separator Low pressure separator Recycle gas compressor Splitter tower with furnace reboiler

2.2.3 Plant 303 - Naphtha Hydrotreating

- Objective: To remove oxygen containing compounds and saturate olefins from the feed to the C5/C6 isomerization and catalytic reforming units. This process is required to meet downstream feed specifications.
- Type: Fixed-bed hydrotreaters
- Selection Rationale:

The process is a commercial technology capable of using catalysts from various manufacturers.

Process Description:

A typical process flow diagram is shown in Figure 2-4. Naphtha from Plant 204 is heated in a fresh feed/reactor effluent exchanger, combined with the makeup and recycled hydrogen, and heated in a single-pass furnace. The hot vapor is sent to a fixed-bed catalytic hydrotreating reactor. Reaction effluent is cooled first via exchanger with the feed, followed by an air fin condenser. The cooled products are flashed into a cold separator.

The separator gas is compressed and recycled back along with the makeup hydrogen to combine with the incoming feed. The separator liquid is charged to a stabilizer column where fuel gas is separated and sent to the saturated gas plant. The bottom from the stabilizer is discharged to a naphtha splitter where the overhead C5/C6 stream is sent to isomerization, and the bottom product stream is sent to the catalytic reformer.

Product Streams:

C5/C6 (303.2) C7+ Naphtha (303.3) Fuel gas (303.1)

Major Equipment/Features:

Reactor Feed/hydrogen furnace Feed/effluent exchanger Air fin condenser Cold separator Gas compressor Stabilizer Naphtha splitter

2.2.4 Plant 304 - Catalytic Reforming

Objective: To increase the octane of the paraffinic heavy naphtha.

Type: UOP's low pressure CCR Catalytic Reformer.

Selection Rationale:

The UOP process is the best way to increase the octane number of straight chained heavy naphthas by converting them to aromatics. A low reactor pressure gives both higher liquid yields and hydrogen production.

Process Description:

A typical process flow diagram is shown in Figure 2-5. The process uses stacked reactors and a Continuous Catalyst Regeneration (CCR) section to maintain a steady state reforming operation at optimum process conditions (i.e., fresh catalyst performance, low reactor pressure and minimum recycle gas circulation.) Slightly aged catalyst is continuously withdrawn from the last reactor and transferred to the regenerator. Withdrawn catalyst is regenerated at steady state conditions and returned to the top of the reactor stack, maintaining near fresh catalyst quality.

Fresh feed (hydrotreated naphtha from both the Naphtha Hydrotreater and Wax Hydrocracker units) is combined with the recycled hydrogen and is preheated. The hot feedstock is charged into the top of the reactor stack. The first reactor stage effluent is reheated before entering the second reactor system. Reheating may occur once or twice more depending on feedstock quality and capacity. Reactor effluent leaving the last reactor stage, heat exchanges with the incoming feed. It is subjected to further cooling, if necessary, before entering the separator. Vapors from the separator are recycled, and the net hydrogen production is sent to the Hydrogen Recovery Plant (Plant 205.) The separator liquid is routed to a fractionation column where the desired C5+ reformate products are separated.

Product Streams:

	C5+ reformate (304.1)
	Hydrogen rich C2- fuel gas (304.2)
	C4-gas (304.3)
Major Equipment/	Features:
· · ·	Catalytic reforming reactor/regeneration system
	Feed/effluent exchanger
	Separator
	Hydrogen recycle compressor
	Fractionation column with heaters

2.2.5 Plant 305 - C4 Isomerization

Objective: To supply a sufficient quantity of isobutane to the alkylation unit by converting inplant and purchased normal butane to isobutane.

Type: UOP Butamer unit.

Selection Rationale:

Two commercial processes are commonly used, namely the UOP butamer process and the BP butane isomerization process. They differ mainly in the type of catalysts employed.

Process Description:

A typical process flow diagram is shown in Figure 2-6. The mixed butane feed (purchased plus inplant) is fed to a deisobutanizer column where isobutane is separated from n-butane. The n-butane feed is mixed with the hydrogen, heated to the reaction temperature, and then fed to the reactor containing a platinum catalyst. The n-butane is isomerized to a nearequilibrium concentration of isobutane. The isomerization products enter a high pressure separator where the unreacted gases are separated from the product, mixed with a small quantity of makeup hydrogen, and are returned to the isomerization reactor.

The liquid product stream passes to a stabilizer where additional dissolved gas is removed. It is then sent to a deisobutanizer column where the desired isobutane product is taken off as the overhead stream and sent to the alkylation unit. The unconverted n-butane is mixed with the fresh feed, and fed to the isomerization reactor.

Product	Streams:	i
		1

iC4 (307.1) Fuel gas (305.2)

Major Equipment/Features:

Reactor(s) Feed preheater Deisobutanizer Stabilizer tower HP separator vessel Hydrogen compressor

2.2.6 Plant 306 - C5/C6 Isomerization

Objective: To convert low-octane (~50-55) straight chained C5 and C6 paraffins to higher-octane (~82-85) branched isoparaffins.

Type: UOP Penex unit.

Selection Rationale:

This is a relatively low cost option to increase gasoline octane. An oncethrough unit is recommended to further reduce the production cost of isomerate. Other commercial processes include that of BP and Shell/Union Carbide. They differ from each other mainly in the catalyst system used and the separation scheme employed to separate the paraffins from the isomerate.

Process Description:

A typical process flow diagram is shown in Figure 2-7. The C5/C6 paraffin feed (Stream 303.2 from the Naphtha Hydrotreating Unit and Stream 301.2 from the Wax Hydrocracker) first is dried over molecular sieves. Then it is mixed with dried makeup hydrogen, steam heated and sent to the fixed-bed isomerization catalytic reactor. Reaction products are passed directly to a stabilizer column after heat exchange. Stabilizer overhead is sent to the Saturated Gas Plant, and the bottom effluent is discharged directly to the gasoline blending storage. The unit has an expected onstream factor of 96%.

Product Streams:

Isomerate (306.1) Fuel gas (306.2)

Major Equipment List:

Reactor(s) Feed drier and preheater Stabilizer Feed/effluent exchanger

2.2.7 Plant 307 - Alkylation Unit

Objective: To convert C3, C4 and C5 olefins into a low Reid vapor pressure (RVP), low aromatic, high-octane gasoline blending stock.

Type: Stratco Inc., technology using sulfuric acid.

Selection Rationale:

This catalytic process was selected because alkylate is a most desirable component for reformulated gasoline. Stratco's technology is chosen for its proven reliability and high yield. An onstream factor in excess of 93% is expected for the process.

Process Description:

A typical process flow diagram is shown in Figure 2-8. F-T products of C3, C4 and C5 olefins from Plant 204 (Stream 204.9 leaving the oxygenate wash tower) along with the makeup and recycled isobutane, and H2SO4 are charged to the alkylation reactor(s) (Stratco Contactor) which contains a mixing impeller and internal cooling tubes. The impeller disperses the hydrocarbon feed with the acid catalyst into an emulsion. The heat of reaction is removed by low-temperature recycle auto-refrigeration which consists of a compressor and a depropanizer.

The reaction product is treated to remove entrained acid by passing through an acid and then a caustic settler. It is then fractionated in the deisobutanizer to remove the isobutane and recycle it to the contactor. The net products consist mainly of normal butane and quality-grade C5+ alkylate.

Product Streams:	nC4 (307.2) C5+ alkylate (307.3) C3- gas (307.4)
Major Equipment List:	Stratco licensed contactors • 5,000 BPSD alkylate, 3 each required • 15,000 BPSD alkylate, 9 each required Flash drum Acid settler(s) Caustic settler(s) Compressor and depropanizer tower Deisobutanizer

2.2.8 Plant 308 - Saturated Gas Plant

Objective: To process and separate saturated gases from various sources within the complex into butane, propane and the C2- fuel gas.

Selection Rationale:

Normal butane is recovered as feed for the C4 isomerization plant, C3 is sold as LPG, and C2- gases are used for fuel gas.

Process Description:

A typical process flow diagram is shown in Figure 2-9. Compressed saturated gas from various sources (i.e., the hydrotreaters, wax hydrocracker, catalytic reformer, the alkylation and isomerization units) are cooled and charged into a deethanizer-absorber. The overhead gas (C2-) is sent directly to the refinery fuel gas system. The deethanized bottoms product is charged into a debutanizer tower. The overhead stream leaving the debutanizer tower is routed to a depropanizer tower where butane and propane LPG are separated. Butane is sent to the C4 isomerization plant. The bottoms liquid stream of the debutanizer goes to gasoline storage.

Product Streams:

nC4 (308.1) C2- fuel gas (308.2) C3 LPG (308.3)

Major Equipment/Features:

Deethanizer absorber tower with intercooler and reboiler

Debutanizer tower

Depropanizer tower Separator

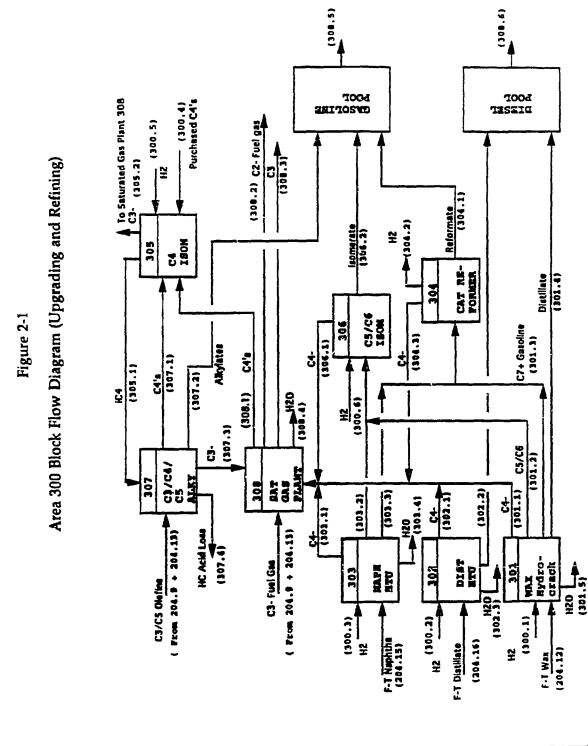
2.3 ALTERNATIVE REFINING CASE

Preliminary design basis for the alternative refining case and the correlation development to predict ZSM-5 conversion and yield were discussed in Quarterly Report Number 3 (April-June 1992), Section 6.2. Work has commenced on this case during this quarter, starting with the modification of the ASPEN/SP code to include the ZSM-5 reactor. This will be reported in Section 3.

The design of the plants in the Syngas Preparation Section remain identical in the Alternative Refining Case to those in the baseline case. Only the plants in the F-T synthesis loop and downstream processing areas are impacted, and many of these plants will be capable of proration.

2.4 WESTERN COAL ALTERNATIVE CASE

Detailed process design information for Area 100 of the Western Coal Alternative Case were reported in Quarterly Report Number 5 (October-December 1992). No further work is planned for this case study until the third quarter of 1993.



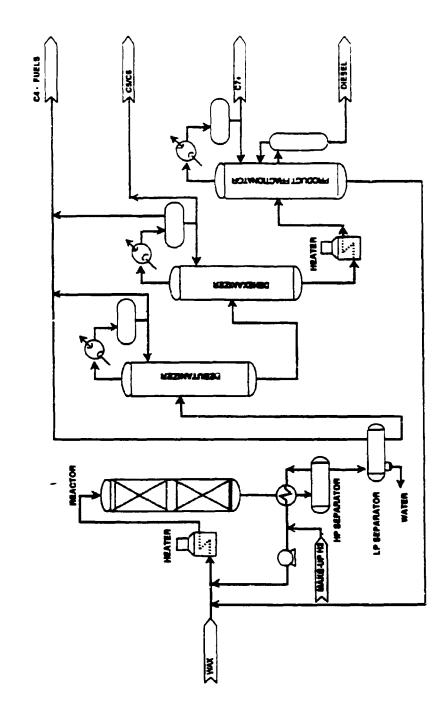
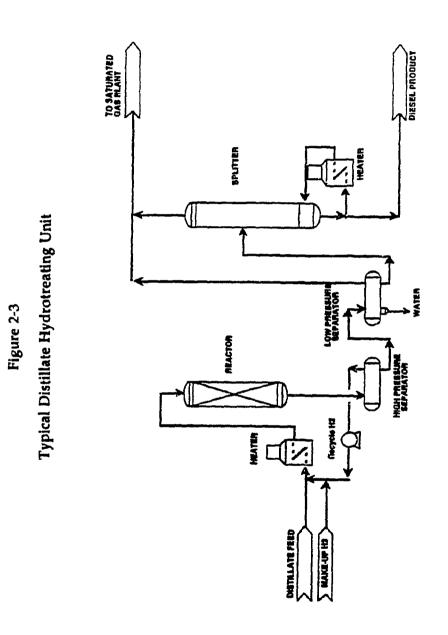
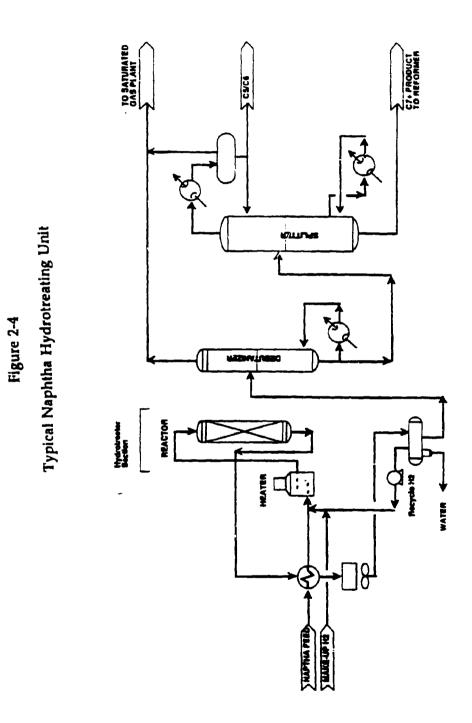
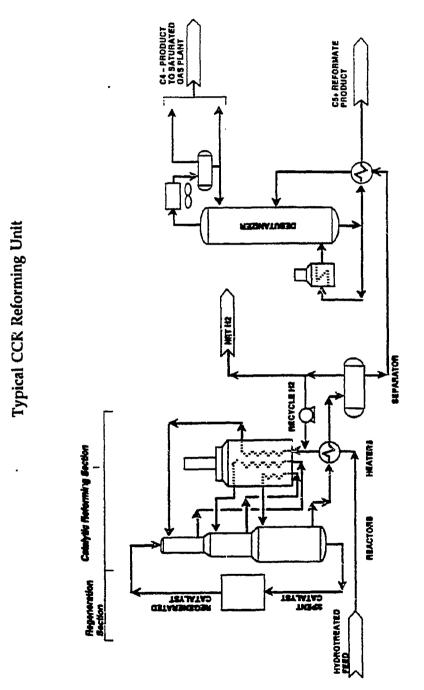


Figure 2-2 Typical Wax Hydrocracking Unit







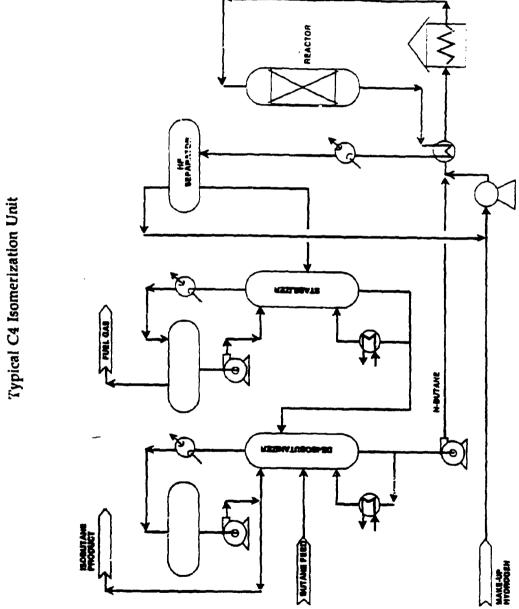
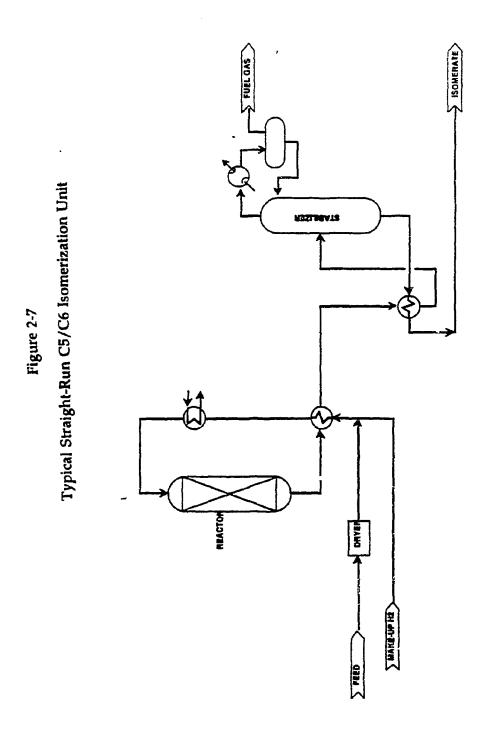


Figure 2-6

Task 1 - Baseline Design and Alternatives



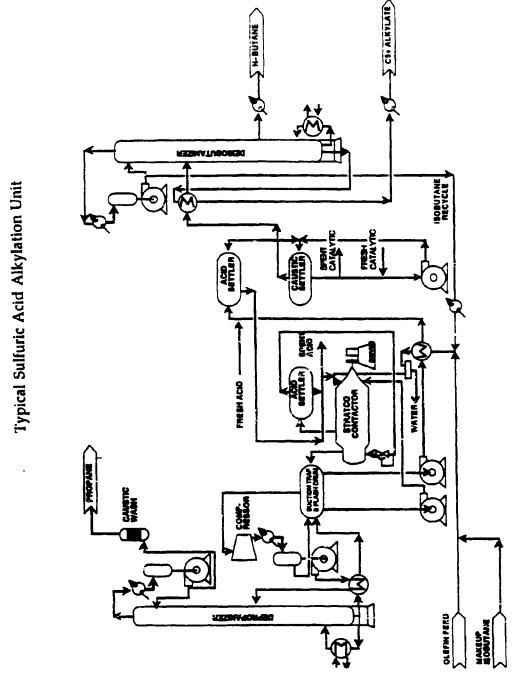


Figure 2-8

Section 2

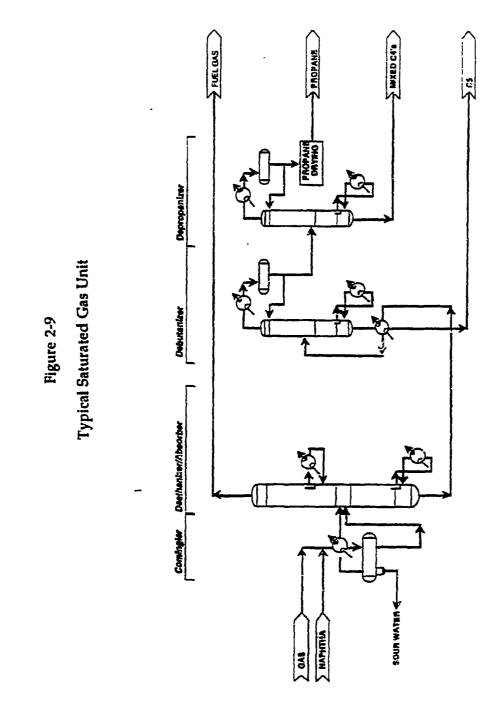


Table 2-1
Material Balance Summary
Plant 201-Flacher Tropach Synthesis
Illinois No. 6 Coal

Stream No.	201.1	201.2	201.3	201.4	201.5	201.6	201.7	
Stream no.	Byngas from eulfur Polishing	Water addition To FT	Feed To F-T Reactor	F-T Vepor	Wax	Aqueous Oxygenates	OH Ges To Fuel	
Phase	Vap	Lig	Vap	Vap	Llq	Llq	Vap	
Component Flows					1			
LBmol/hr		1]			
H2	33,295.00		46,773.00	13,804.00	0.61	0.00	3.20	
N2	965.08		3,457.49	3,456.57	0.14		0.71	
02			1					
00	92,245.00	1	101,100.00	13,219.00	0.57	0.00	3.0	
CO2	3,816.68		6,011.58	54,000.00	10.26	2.19	23.1	
H2O	472.75	5,405.00	11,092.00	2,231.46	2.99	1,820.51	1.6	
CH4	22.88		463.29	1,424.09	0.14	0.00	0.4	
C2H4			0.02	392.01	0.09		0.1	
C2H6		[0.02	98.20	0.03		0.0	
C3H6				348.34	0.20	1	0.2	
C3H6		1	1	61.47	0.04		0.0	
ICAHS		1		13.6 0	0.02	}	0.0	
NC4H6		1]	258.08	0.30		0.1	
IC4H10		1	1	3.39	0.00		0.0	
NC4H10				64.51	0.08		0.0	
C5H10				211.00	0.40		0.1	
IC5H12				7.03	0.01		0.0	
NG5H12				0 3.27	0.15		0.0	
C6H12			1	174.86	0.88		0.1	
IC6H14				5.83	0.02		0.0	
NC6H14				52.44	0.22		0.0	
C7-C19				986.82	51.74	l	0.1	
WAX				3.00	457.97			
OXVAP				43.51	0.10	0.32	0.0	
OXHC				159.22	1.41		0.0	
OXH2O				159.46	0.36	159.46	0.0	
Catalyst								
Total	130,817.39	5,405.00	164,797.36	91,242.01	528.51	1,982.49	33.6	
Totel ib/hr	2,854,800	97,372	3,490,500	3, 194, 700	294,540	40,175	1,252	
Mol. Wt.	21.82	18.02	20.68	35.01	557.31	20.26	37.1	
MINSCED	1,191.48		1,537.41	831.03		1		

Table 2-1 (Cont.) Material Balance Summary Plant 201-Fischer Tropach Synthesis Illinois No. 6 Coal

Stream No.	201.8	201.9	201.10	201.11	201.12	201.13
	Water For Oxyg Wash	Aqueous Water To Treatment	HC Liquid	Unconverted Synges	Pretreated Catalyst To F-T	Waste Catalyst To Disposal
Phese	Liq	Llq	Llq	vap	Sturry	Solid
Component Flows						
LBmol/hr						
H2		0.57	5.42	13,798.00		
N2			2.00	3,454.23		
02		l l				
00		0.35	8.65	13,210.00		
CO2		0.00	333.81	53,6 84.00	1	
H2O	1,200.00	1,200.00	43.48	367.42	l	
CH4		0.03	2.41	1,421.65		
C2114			2.25	390.55		
C2H6			0.80	97.40	ľ	
C3HC			7.51	340.82		
C3H9			1.52	59.95		
IC4H8			0.82	12.77		
NC4H8			15.81	242.25		
104110			0.16	3.22		
NC4H10			4.58	59.94		
C5H10			30.38	160.62		
IC5H12			1.04	5.99	1	
NC5H12			11.52	51.76		
C6H12)	60.52	114.34		
IC3H14			1.86	3.97		
NC6H14			20.12	32.32		
C7-C19 WAX		1	861.35	125.45	4050 051	
OXVAP		27.81	3.09 15.30		1652.25	24.28
OXHC		21.01	141.49	17.73		
OXH2O		l	141.48	17,73		
Catalyst					470 70.	470 70
Total	1,200.00	1 000 77	1,675.95	07.054.00	479.75	479.75
Total Ib/hr	21,618	1,228.77	1,675.95	87,654.36		~ ~
Mot. Wt.	18.02	23,052 18,76	173,870	2,979,200	2132	50
MMSCFD	10.02	10.70	110.33	33.99 798.30	l	
	("Indicates flow in	بالبيب ويسو				

("Indicates flow in ib/hr; Catalyst replacement rate is 11,514 lb/day)

Table 2-2Material Balance SummaryPlant 202-CO2 RemovalIllinois No. 6 Coal

Stream No.	202.1	202.2	202.3	202.4
	Unconverted	Deethanizer	Recycle Gas	Scrubbed
	Syngas	Overheed	To	coz
	From F-T	Vapor	Compressor	
Phase	Vap	Vap	Vap	Vap
Component Flows				
Lbmol/hr				
H2	13,798.00	17.42	13,815.00	
N2	3,454.23	20.49	3.474.72	
02				
8	13.210.00	94.55		
CO2	53,664.00	484.57	270.74	53,878.00
H20	367.42	0.00		
CH4	1.421.65	56.38		
C2H4	390.55	238.49	_	
C2H6	97.40			
C3H6	340.82	16.95		
Сзня	59.95	1.79		
IC4H8	12.77		12.77	
NC4H8	242.25		242.25	
IC4H10	3.22		3.22	
NC4H10	59.94		59.94	
C5H10	180.62		180.62	
ICSH12	5.99		5.99	1
NC5H12	51.76	1	51.76	
C6H12	114.34		114.34	
IC6H14	3.97		3.97 32.32	
NC6H14 C7-C19	32.32 125.45	•	125.45	
WAX	123.43		123.43	
OXVAP		1		
OXHC	17.73		17.73	
OXH2O	11.73	5	17.73	
UXH2U				
Total	87,654.36	1,046.88	34,823.44	53,878.00
Totel Ib/hr	2.979.200	36,460	644,520	2,371,100
Mol.Wt	33.59			44.01
MMSCFD	798.36	9.53	317.17	490.72

Table 2-3Material Balance SummaryPlant 203-Compression & DehydrationIllinois No. 6 Coal

Stream No.	203.1	203.2	203.3	203.4	203.5	203.6	203.7
	Syngas From	Liquid	Synges To	Water To	Unused Fuel	Fuel Gas From	Total Fust Gas
	CO2	Hydrocarbons	Hydrocarbone	Waste	Gas From H2	H2 Recovery/	To
	Removal	To Desthanizer	Recovery	Treatment	Recovery	Regeneration	Gas Header
Phase	Vap	, Liq	Vap	Liq	Vap	Vap	Vap
Component Flowe		·					
LBmol/hr							
H2	13,815.00	0.57	13,815.00		1,306.95		2955.5
N2	3,474.72	0,22	3,474.50		428.27	540.23	968.4
02							
00	13,305.00		13,304.00		1,037.95		3704.0
CO2	270.74		270.52		14.50	18.30	
H2O	367.42			267.71			92.1
CH4	1,478.03				207.51		
C2H4	629.04		628.56		48.55		
G2H6	213.64		213.41		56.42	71.17	
C3H6	357.77		356.69		3.25	4.10	
C3H8	61.74		61.53		0.45	0,56	
icaho	12.77		12.66		0.01	0.02	
NC4H8	242.25		239.99		0.22	0,28	
IC4H10	3.22		3.19		0.00	0.01	0.0
NC4H10	59.94	0,65	59.29		0.04	0.05	
CSIIIO	180.62		176.04		0.02	0.02	
IC5H12	5.99		5.64				0.0
NC5H12	51.78		50.08		0.00	0.00	
C6H12	114.34		105.54				0.0
IC6H14	3.97		3.70				
NCEH14	32.32		29.46				
C7-C18	125.45	39.91	85.54				
WAX	c .		1				
OXVAP	-						
OXHC	17.73	11.04	6.69				
OXH2O							
Total	34,823.44	84.13	34,379.98	267.71	3,704.14	4,672.48	8,468.7
Total Ib/hr	644,230		630,340	4,812	68,443		154,77
Mol. WL	18.50		18.33	17.97	18.48	19.40	18.2
MEASCED	317.17	1 1	313.13		33.74	42.56	77.1

Table 2-4 Material Balance Summary Plant 204-Gas Plant Illinois No. 6 Coal

Stream No.	204.1	204.2	204.3	204.4	204.5	204.6	204.7
	Byngae	Syngae	HC Liquide	HC Liquide	HC Liquids	Side Water	Deethanizer
	To	From	To	From	From	Draw From	Overhead
	H2 Recovery	Dehydration	Desthenizer	Compr & Dehy	F-T Reactor	Deethanizer	Vapor
Phase	Vilip	Vep	Ĺlq	Liq	Liq	μų	Vap
Component Flow		,t					
Lbmol/hr							
H2	13,003.00	13,815.00	11.43		5.42		17.42
N2	3,456.31	3,474.50	18,19	0.22	2.08		20.46
02							
00	13,219.00	13,304.00	84.97	0.93	8.65	0.00	94.54
CO3	117.08	270.52	153.40		333.81	1.53	485.26
H20				7.59	43.48	0.12	56.37
CH4	1,424.06	1,477.74	53,68		2.41	0.01 0.59	238.63
C2H4	391.84	828.58	238.74		2.25		117.8
C2H6	92.34	213.41	121.07	0.23	0.80	0.73	16.83
C3H6	20.20	350.89	330.44	1.08	7.61	1.20	1.72
C3H8	3.60	61.53	57.93		1.52	0.19	1.74
104118	0.10	12.66	12.50	0.12	0.82	0.03	
NC4HB	1.78	239.99	238.21	2.26	15.81	0.65	
IC4H10	0.04	3.19	3.15	0.02	0.18	0.01	
NC4H10	0.33	59.29	66.9 7	0.65	4.56	0.16	
CSH10	0.13	176.04	176.01	4.58	30.38	0.50	
IC5H12	0.01	5.84	5.83		1.04	0.02	
NC5H12	0.02	50.0 8	50.05		11.52	0.15	1
C6H12	0.01	105.54	105.54		60.52	0.40	
IC6H14		3.70	3.70		1.80	0.01	
NC6H14	0.00		29.46	2.66	20.12	0.12	
C7-C19		85,54	85.54	39.01	861.35	2.20 0.01	
WAX					3.09	0.01	
OXVAP					15.30		
OXH2O		6.69	6,69	11.04	141.49	0.35	
Total	32,035.07	34,370.98	1,843.52		1,575.95	9.00	1,049.06
Total Ib/hr	538,080	630,600	92,514	-	173,870	665	36,547
Mol, WL	10.54	18.34	50.18	88.49	110.33	73.95	34.84
MMSCFD	296.34	313.13					9.56

Table 2-4 (Cont.) Material Balance Summary Plant 204-Gas Plant Illinois No. 6 Coal

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Stream No.	204.8	204.9	204.10	204.11	204.12	204.13	204.14
	Water	HiC Llq	Aqueous H2O	Depentenizer	Feed To	Fractionator	Condensate
	To OXHC Wash	To	То	Underflow	Product	Overhead	To water
	Column	Alkylation	Treatment		Fractionator	To Alkylation	Treatment
Phase	Liq	Llq	Liq	Liq	Liq	Vap	Llq
Component Flow		ī,1					
Lbmol/hr	[]			•			
H2	[[0.81	0.61	I
N2	1 1				0.14	0.14	
02	1 1						
00	1 [0.57	0.57	
CO2		0.71			10.26	10.26	
H2O	600.00	4.55	846.04	0.35	3.34	3.34	1,700.00
CH4	{ {				0.14	0.14	
C2H4		0.23			0.09	0.09	
C2H6	1 1	3.56			0.03		
C3H6		320.99		0.02		0.22	
C3H8		57.74		0.01	0.04	0.04	
IC4H9		13.42		0.03	0.04	0.04	
NC4HB		254.99		0.52		0.82	
IC4H10		3.34		0.00		0.01	
NC4H10		63.75		0.23			
C5H10	1 1	199.85		10,62			
IC5H12		6.37		0.64	0.65		
NC5H12	1	12.62		50.48	50.83	10.08	
C6H12		•		174.46	175.11		
IC6H14				5.82	5,84		
NC6H14				52.32	52.53		
C7-C19				984.61	1,036.35		
WAX]]			3.08	461.06		
OXVAP	1		15.26				
OXHC				158.87	160.28		
OXH2O							
Total	600.00	942.15	661.30	1,441.93	1,969.98	38.23	1,700.00
Total Ib/hr	10,812	50,628	12,416	184,373	478,378	2,157	30,63/
Mol. WL	18.02	53.74	18,77				18.02
MMSCFD	ļ					0.35	

Table 2-5Material Balance SummaryPlant 205-Hydrogen RecoveryIllinois No. 6 Coal

Stream No.	205.1	205.2	205.3	205.4	205.5
	H2 From Cat.	Recycle Ges	H2 Product	Fuel (Purge)	Autothermal
	Reformer	From	From	Ges	Reformer
	Area 300	Plant 204	PSA		Feed
Phase	Vap	Vap	Vap	Vap	Vap
Component Flows					
Lbmol/hr					
H2	2,127.97	13.803.00	3,040.29	2955.56	9,935.59
N2		3,456.31		968.49	2.487.81
02					
ω		13,219.00		3704.08	9,514.86
CO2		117.06		32.80	84.26
H2O					
CH4	70.23	1,424.06		469.27	1,025.02
C2H4		391.84		109.80	
C2H6	101.71	92.34		127.58	
C3H6	j i	26. 26	1	7.36	18.90
СЗН8		3.60	3	1.01	2.59
IC4H8		0.10	1	0.03	
NC4H8		1.78	1	0.50	
IC4H10		0.04		0.01	0.03
NC4H10	1	0.33		0. 09	
C5H10	1	0.13		0.04	
IC5H12		0.01		0.00	
NC5H12		0.02		0.01	-
C6H12	1	0.01	ł	0.00	0.01
IC6H14		l.	[
NC6H14					0.00
C7-C19		1	1		
WAX		ł			
OXVAP					ļ i
OXHC	1			1	1
OXH2O		1			ł
Total	2,299.91	32,535.87	3,040.29	8.376.62	23.419.28
Total Jb/hr	8.472				5
Mol. WL	3,66				1
MMSCFD	20.95				

Table 2-6

Material Balance Summary Plant 206-Autothermal Reformer Illinois No. 6 Coal

Stream No.	206.1	206.2	206.3	206.4
	Oxygen	Steam	Syngas	Recycle Gas
	Addition To	Addition To	From	To
	Reformer	Reformer	H2 Recovery	F-T Reactor
Phase	Vap	Vap	Vap	Vap
Component Flows				
Lbmol/hr				
H2			9,935.59	13,478.00
N2	4.59		2,487.81	2.492.41
02	314.04			
ω			9.514.86	8,857.35
CO2			84.26	2.094.88
H2O		6.750.00		5.214.35
CH4			1.025.02	440.41
C2H4			282.05	0.02
C2H6			66.47	D.02
C3H6			18.90	
C3H8			2.59	
IC4H8			0.07	
NC4HB			1.28	
IC4H10			0.03	
NC4H1G			0.24	
C5H10			90.0	
IC5H12 NC5H12			0.00 0.02	
CSH12			0.02	
IC6H14			0.01	
NC6H14			0.00	
C7-C19			0.00	
WAX				
OXVAP				
OXHC				
0X1-20				
Total	918.63	6.750.00	23,419.28	32.577.42
Total Ib/hr	29,377	121,600	387,310	538,290
Mol. Wt.	31.98	18.01		16.52
MISCED	8.37	61.48	213.30	296.72

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	Table 2-7 (1)
Area	300 -Product Upgrading and Refining
	Material Balance Summary

	Area 300 -Product Upgrading and Relining Material Balance Summery										
	Naphthe Hydrotreeting Distillate Hydrotreeting										
	Feed	H2 Required	the second s	(:5/C6		1120 Prodoed	Feed	H2 Required		Diesel	
Component	204.18	300.5	903.1	303.2	E, EOE	303.4	204.14	300.2	\$02.1	302.2	
H2	1	1472		0	0			727	0	Q	
N2	0		0	0	0		0		0	0	
00	0		0	0	0		0		0	0	
002	0		0	o	0		2		0	0	
H2O	(O		,i O	Q	0.		0		85	0	
CI	0		360	0	a		0		0	0	
C2-	ð		0	0	0 0		ő		128	ŏ	
C2	0		1342	0	0		0		0	Ő	
C3-	0		0	0	C C		0		298	0	
C3	0		1711	0	с 0		0		128	0	
K4	0		240 1144	0	0		0		213	0	
nC4 C4=	0		0	0	0		ŏ		D	ő	
C4= IC5	2		ů	76	0		ŏ		0	ō	
nC5	2022		ă	3672	ō		ŏ		ō	ō	
C6-	0		ŭ	0	0				ō	ō	
C 6	14737		ů v	ŏ	ō		ō		Ō	Ō	
ica .	603		ŏ	2013	ō		ō		0	0	
n C6	4527		õ	10110	ō		Ö		0	0	
C7-C10 (Nephthe)	69758		Ō	0	Ö		0		0	0	
C11-C19 (Distillate)	0		0	0	0		05112		0	0	
C18+ (Wax)	0		0	0	0		0		0	0	
180-300OX	8782		0	0	0		0		0	0	
300-350OX	709		0	0	0		0		0	0	
350-700OX	0		0	0	0		8341		0	0	
Reformate	0		0	0	0		0		0	0	
C3 Alkyinte	0		0	0	0		0		0	0	
C4 Alkylate	0		0	0	0		0		0	0	
C5 Alighte	0		0	0	0		(0		0	0	
CS loomers.lo	0		0	0	0		0		0	0	
C8 isomerale	0		0	0	0		0		0	0	
C7-300 HC	0		0	0	0		0		0	0	
300-350 HC	. 0		0	0	0		0		0	0	
350-500 HC	0		0	0	0				U 0	0	
500-700 HC	0		0	0	0 54873	1	0		0	0	
C7-300 HTU 300-380 HTU			0	0	15583				ŏ	0	
360-380 HTU	0		0	0	0		ŏ		ŏ	54494	
500+ HTU	ŏ		ő	Ö	õ		0		õ	36026	
H2O Produced	ő		ŏ	ŏ	ō	2368	ŏ		ŏ	g	
Total (LMAr)		1478	4788	23778	70488	2368	01484	727	851	00820	
Totel (BPSD)	8610			2401	6884	102	8085		105	8134	
Density (19/113)	44.4384		31.2835	40.0000	44.2868	62.2978	40.2077		34.4807	47.5622	
Moi. Wt	100.34	2.02	37.00	83.88	117.88	10.02	192.80	2.02	38.40	102.40	

Table 2-7 (2) Area 300 -Product Upgrading and Refining Material Balance Summary

		<		Wax Hydrocr				**************************************	« ************************************	
	H2O Produced	Feed	H2 Required	C4-	C5/C6's	C7+ Naphtha	Distillate	H2O Produced	Olelin Feed	C4 Mahoup
Component	302.3	204.12	300.1	301.1	301.2	301.3	301.4	301.6	204.9+204.13	305.1
H2			3845	Ō	0	0	0		0	0
N2		0		0	0	0	0		0	0
00	1	0		0	0	0	0		0	0
CO2	1	0		0	0	0	0		a	0
H2O		0	۱,	0	0	0	0		0	0
C1		0		141	0	0	0		0	0
C2=)	0		0	0	D	0		0	0
C2		Ċ		141	0	0	0		0	0
C3=		Û			0	0	0		13518	0
C3		0		4187	0	0	0		2546	0
IC4	1	0		5546	0	0	0		195	46358
nC4	1	0		4500	0	0	0		3725	1929
C4=		0		s	0	0	0		15108	0
iC6	1	0		0	6903	0	0		604	0
nCō		0		0	5830	0	0		1641	0
C5=	1 1	0		0		0	0		14782	0
C6=	1	0		0	0	0	0		0	0
ica	1	0		0	10978	0	0		0	0
nC6		0		0	6734	0	0		0	0
C7-C10 (Naphtha)		0		0	O	0	0		0	0
C11-C19 (Distillate)	1	0		0	0	0	0		lo	0
C19+ (Wax)		284845		0	0	0	0		0	0
160-300OX		0		0	0	0	0		0	0
300-350OX		0		0	0	0	0		0	0
350-700OX		0		0	0	0	0		0	0
Reformate	1	0		0	0	0	0		0	0
C3 Alkyiste		0		0	0	0	0		0	0
C4 Alkyinte		0		0	0	0	0		0	0
C5 Alkyine		0		0	0	0	0		0	0
C5 isomeraie		0		0	0	0	0		0	0
Cő isomerale	1	0		0	0	0	0		0	ð
C7-300 HC		0		0	0	40972	0		0	0
300-350 HC] (0		0	0	13157	0		Ó	0
350-500 HC	}	0		0	0	0	59989		0	0
500-700 HC		0		0	0	0	127703		ō	Ō
C7-300 HTU		0		0	0	0	0		0	0
300-350 HTU		0		0	0	Ó	0		o	Ō
360-600 HTU	1	0		0	0	0	0		ō	Ō
500+ HYU		0		0	Ō	Ō	Ō		ō	ō
H2O Produced	809	0		Ō	0	Ō	Ō	1910	ō	ō
Total (LM/hr)	808	284848	3845	14814	30445	\$4130	187692	1010	52020	40208
Total (SPSD)	50	20928			3238	6127	10520	131	6116	5880
Deneity (Ib/ft3)	62.2978	58.1778			40.2197	44.2042	40.5501	62.2078	36.3552	38.1005
Mol. WI	18.02	617.82	2.02	\$1.61	79.70			18.02	54.40	60.12

	C4's	Altylation	C3.	HC Acid Loss		H2 Required	Fuel Ges	C4.	Isomerale	H2 Required
Component	307.1	307.2	307.3	307.4	300.4	300.8	305.2	306.1	306.2	300.6
HI2	0		0		0	22	0	0	0	77
N2	Ö	ō	Ō		0		0	0	0	
œ	ŏ	ă	ō		0		0	0	0	
002	ō	0	0		0		0	0 ·	0	
H2O	ŏ	ō	ā		0		0	0	0	
C1	ō	0	1 0		ìo		92	40	٥	
C2-	ŏ	D	Ō		ō		0	0	0	
C2	ā	ō	ō		ō		207	18	0	
C3-	Ö	ō	Ō		ō		0	1	Ð	
C3	ō	ō	2548		ō		561	041	0	
ici		0	0		1325		0	200	0	
nC4	5654	ŏ	ŭ		25178		ō	0	0	
C4=	0	ő	ō		0		ō	0	0	
iCs	ŏ	504	0		1 -		ō	0	D	
nC5	ŏ	1841	ő		0		0	0	0	
C5-	ŏ	0	ō		Ö	•	o	0	0	
C 6 =	ŏ	0	ŏ		Ö		0	6	0	
K6	ō	ŏ	õ		ā		Ō	Ö	0	
nCA	ŏ	ŏ	ō		ŏ		Ō	0	0	
CT-C10 (Nephtha)	ŏ	ŏ	õ		ö		Ď	Ō	0	
C11-C19 (Uiutiliate)	ŏ	Ň	ō		ŏ		ō	l o	D	
C19+ (Wax)	ŏ	ŏ	ő		i i		0	0	0	
180-300OX	ă		ň		ä		Ō	Ó	0	
300-350OX	ŏ	ů n	ŏ		ō		ō	0	0	
350-700OX	ŏ	ő	Ň		à		ō	l o	0	
Reformale	ŏ	ŏ	ő				ō	l o	0	
C3 Aliginte	ő	32186	0				0	6	Ō	
C4 Allyinia	ő	30050	ŏ				ō	ŏ	Ō	
		25863	å	1			ō		õ	
CS Alloyiste	ů ů	20043	<u> </u>				ŏ	0	16100	
Cő leomerale	ő	0					ŏ	l õ	37198	
C6 learnerate	0						ŏ	l õ	0	
C7-300 HC 300-350 HC	ů	U O	ů 0				ŏ	ő	õ	
•••••••••••••••••••••••••••••••••••••••		0	0				õ		ō	
360-500 HC	Ď				ő		õ		Ő	
500-700 HC	0	0	0				0		å	
C7-300 HTU	0	ů	0				0		ŏ	
200-350 HTU	0	D	0		0		ŏ	ő	ő	
350-500 HIU	0	0	0		0		ŏ		ŏ	
500+ HTU	0	0	O D	944	ő		0		ő	
H2O Produced		•	2548	944	20003	22	880	1008	83296	77
Total (Lb/hr)	5054	# 11 # 1	1.44	***	3110			1	5601	••
Total (SPOD)	004 30.3070	8810 44.2237	\$1.5050		36.3133		31.7323	34.0043	40.0710	
Deneity (Ib/Its)	30,3070	44,2237	31.0000		30.3133		31.7323	100 27	#1 AG	2.02

88.12

2.02

100.27

53.92

81.40

2.92

Table 2-7 (3) Area 3@ -Product Upgrading and Refining Material Balance Summary

Density (Ib/NS) Mol. WI

88.12

108.45

44.10

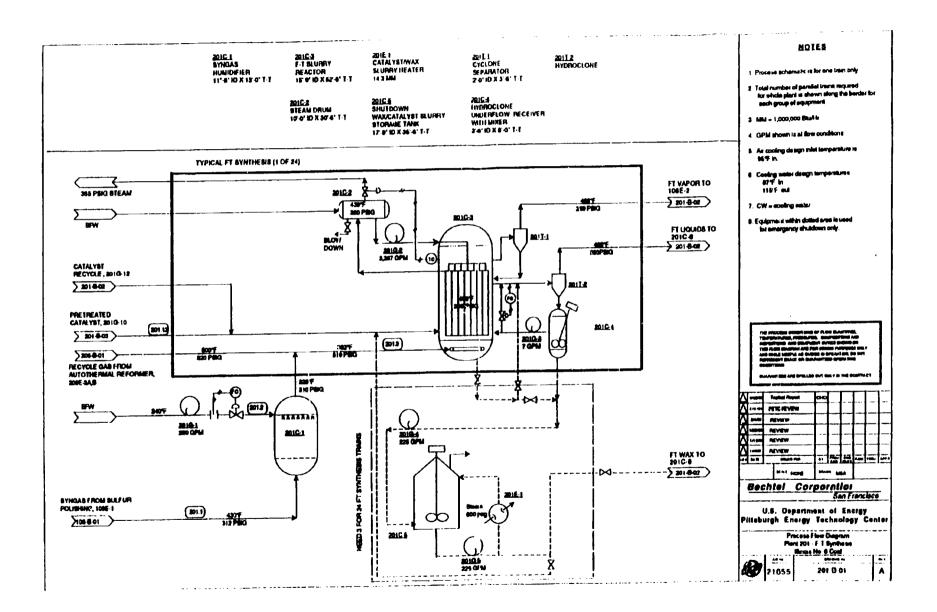
Table 2-7 (4)

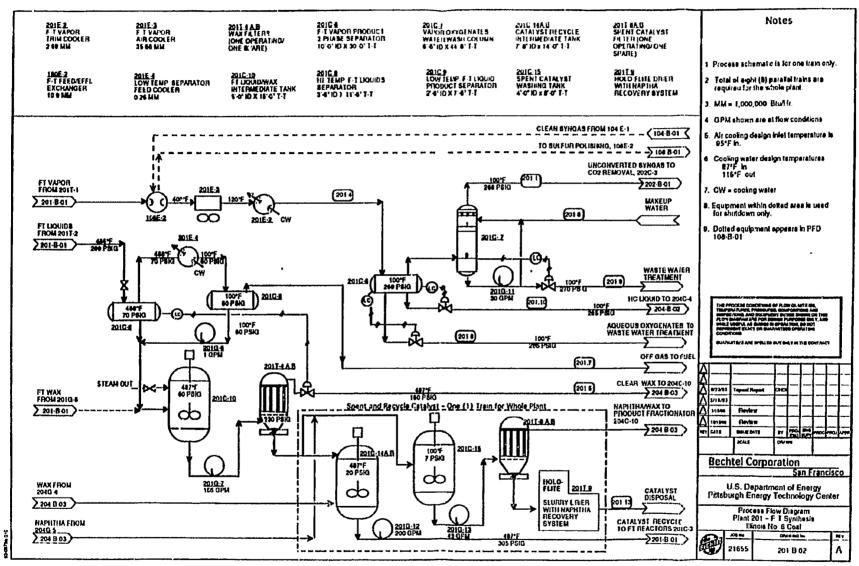
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Area 300 -Product Upgrading and Relining Material Balance Summary

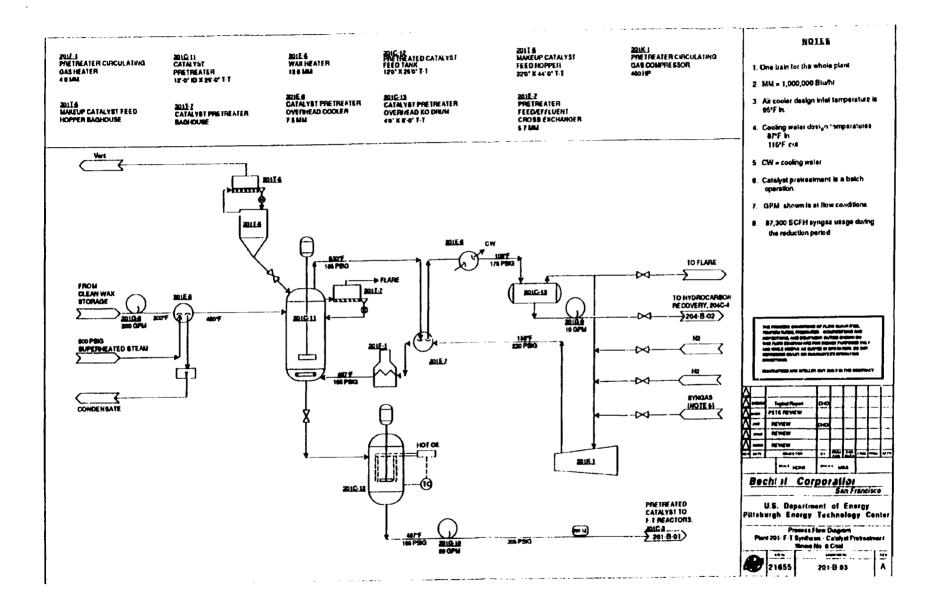
	Catalyti Reformate	H2/C2-	C3/C4	C4'9	Baturated Ga	C3	H20	Fuel Gas From	Gashine	Diesel
Component	304.1	304.2	304.3	308.1	108.2	308.3	308.4	204.9+204.13	308,5	308.6
H2	0	4288	0	0	1	0		1	ō	0
N2	ŏ	0	ō	0	4	0		4	0	0
8	lo	ō	ō	D	16	0		18	0	0
002	ō	ō	0	ō	483	0		483	0	0
H2O	ō			õ	0	0	142	142	O	0
Ci	ō	1126	, U 0	0	719	0		2	6	0
C2=	Ō		ō	0	9	0		9	0	0
C2	lõ	3057	Õ	0	1903	39		108	0	0
C3=	ō	••••	õ	ō	0	0			0	0
C3	ŏ	0	3887	ō	0	13832			0	0
ic.	ō	Ö	2337	8379	Ō	171			0	0
nC4	å	ő	2908	8589	õ	175			0	0
C4=	0	ŏ	0	0	ō	0			0	0
iC5	Ö	õ	ŏ	ō	ŏ	Ō			504	0
nC5	l õ	ŏ	ŏ	ō	Ō	ō			1841	0
C5=		ů	õ	Ö	D	ō			O	0
C6=	0	0	ŏ	Ö	õ	Ō			0	0
iC6	ő	Ő	õ	ŏ	ŏ	Ō			0	0
nC6	ŏ	Ŭ	ő	ŏ	ŏ	ō			ā	0
C7-C10 (Naphtha)		8	Ö	Ö	ŏ	· Õ			0	D
C11-C19 (Distillate)	Ö	0	Ğ	0	ŏ	ō			0	0
C19+ (Wex)		ð	0	Ö	õ	ō			0	Ō
160-300OX		Ű	ŏ	ŏ	ŏ	ō			Ō	0
300-350OX	l o	0	ŏ	ŏ	D	ō			0	Ó
350-700OX		õ	õ	ŏ	ō	õ			Ō	0
Reformate	105962	0	D	ŏ	õ	ō			106982	0
		ŏ	ŏ	ŏ	ŏ	ŏ			32196	Ō
C3 Alkylete	0	0	0	å	õ	õ			30956	0
C4 Alkyinte		0 O	0	l o	ŏ	õ			25863	0
C5 Alkylate		0	0	ŏ	0	Ö			16100	ō
C5 isomerale	0	0	0	o	Ő	0			37196	ŏ
C6 fromerate	Ö	+	0	ő	0	0			0	ŏ
C7-300 HC	0	0	0	0	0	0			õ	ŏ
300-350 HC		-	D	ŏ	0	0			Ŭ	59989
350-500 HC	0	0	0	ő	0	0			õ	12770
500-700 HC	0	-		Ö	G	0			õ	0
C7-300 KTU	0	0	0	0	0	0 0			Ğ	ŏ
300-350 HTU	0	0	U G	0	0	0			Ő	54494
350-500 HTU	0	-	-	0	0	0			D	36026
500+ HTU	0	0	0	0	U Q	0			0	0
H2O Produced	0	0	0	-	-	14217	142	765	251430	27821
Total (LM/hr)	108002	8472	0132	14068	3138	1421/ 1921	142	/ • •	23916	24855
Total (BP\$D)	8804		11//3	2051		1#Z1 31.6382	42. 29 78		44.9354	42.229
Density (ib/it3)	40.1082		33,4653	38,7141						48.220
Mol. WI	1	3.68	\$1.19	80.12	28.48	44.30	10.DZ			

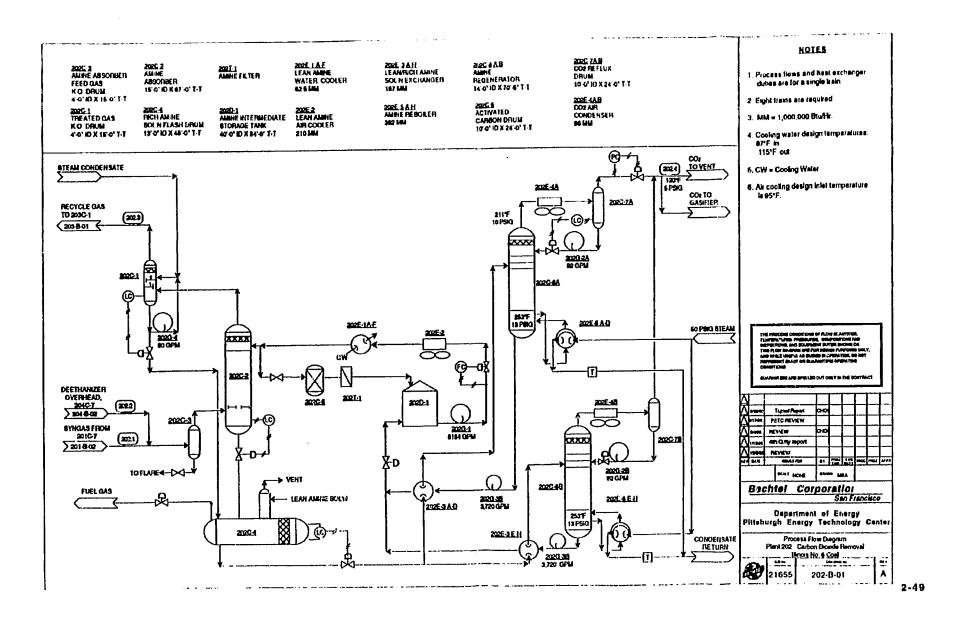
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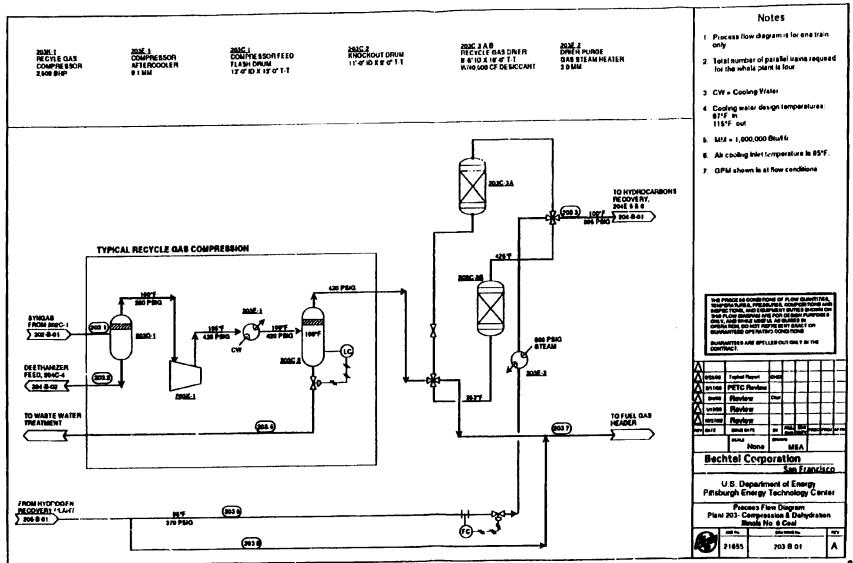




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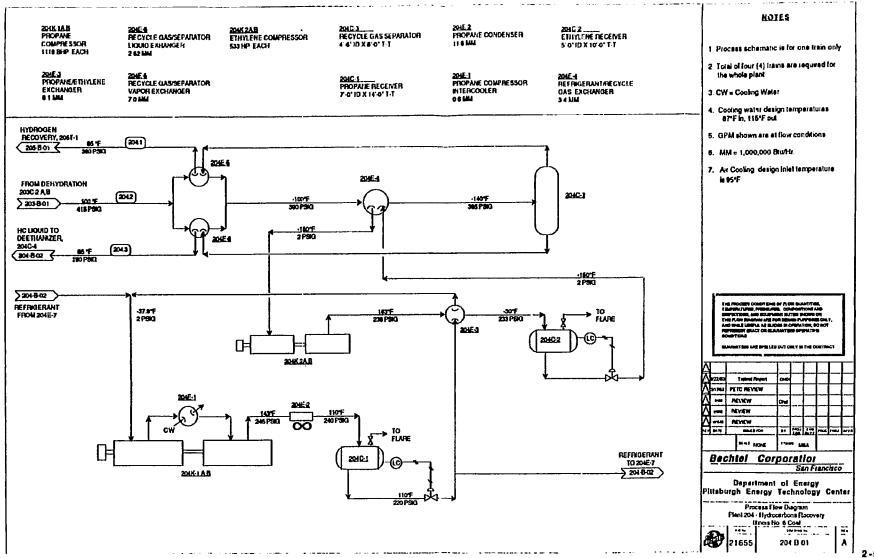


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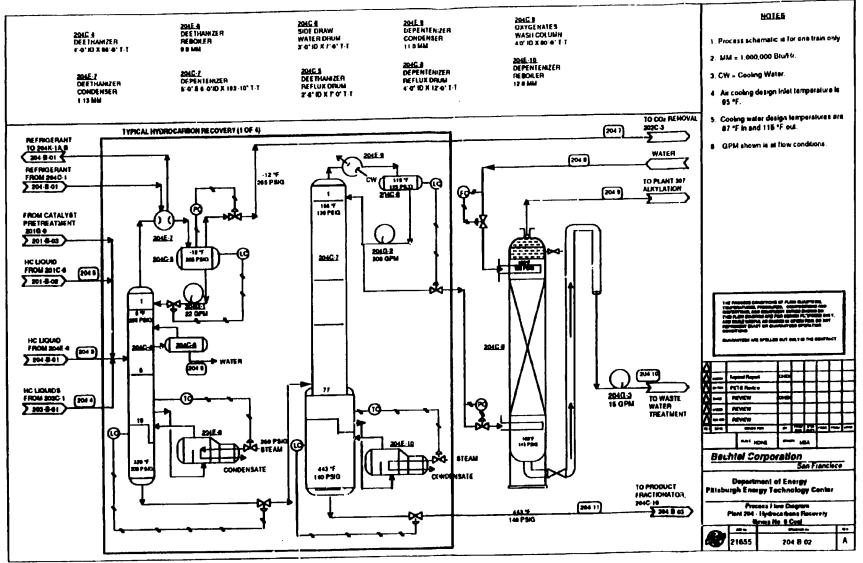
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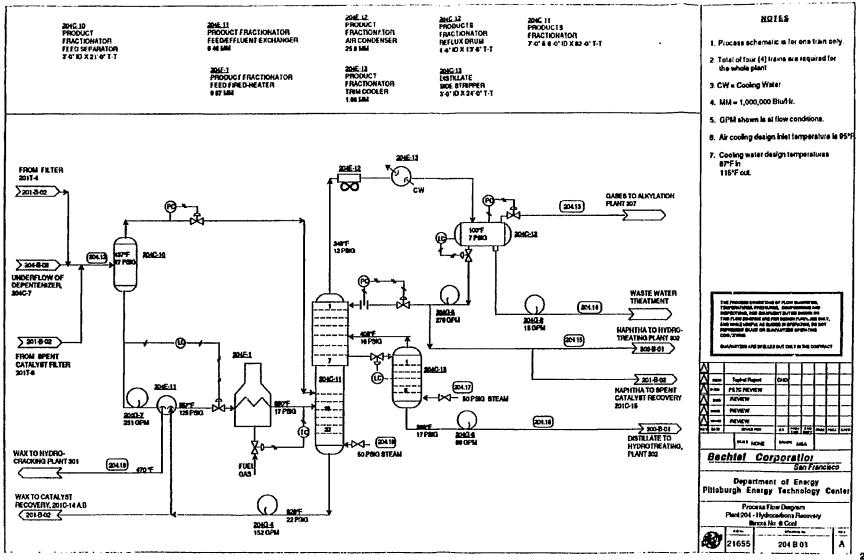
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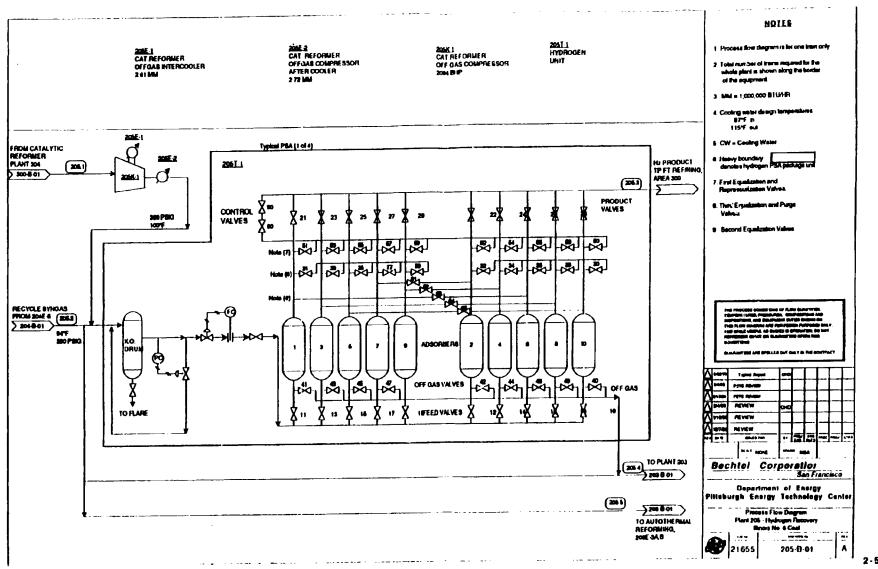
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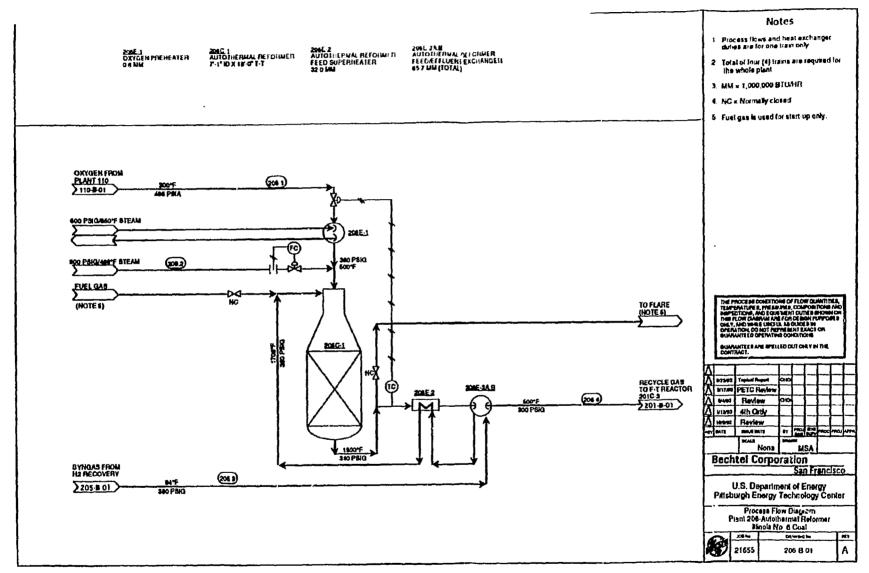


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Section 3

Task 4 - Process Flowsheet Simulation (PFS) Model

Previous quarterly progress reports described the development of a preliminary process simulation model for the Area 100 syngas production section of the plant, an equilibrium gasifier model, and a preliminary Fischer-Tropsch reactor loop (Area 200) model. During this quarter the Fischer-Tropsch reactor loop model was expanded and enhanced, and individual plant models were developed for all the units in the Area 300 product refining section.

3.1 AREA 200 FISCHER-TROPSCH SYNTHESIS MODEL

The preliminary version of the ASPEN/SP Fischer-Tropsch reaction loop model, which was developed by Bechtel, was simplified by removing two convergence loops to reduce the execution time (since the as-received model took over five hours to run on a Compaq 386/33 machine). The major simplifications involved removing two loops that balanced heat exchanger duties and replacing them with fixed temperature specifications. Although these loops are important in developing an economic engineering design, they are not critical for predicting overall plant performance.

Figure 3-1 shows the block flow diagram for the simplified ASPEN/SP model of the Area 200 section of the plant, the Fischer-Tropsch loop. The stream and processing blocks will be renamed later to conform to the model naming conventions. This simplified model new has only one convergence loop and executes in about 15 minutes on the Compaq 386/33 machine.

This model was enhanced by the addition of a ZSM-5 oligomerization reactor that can process all the vapor leaving the Fischer-Tropsch reactors so that the alternate refining case may be studied.

3.1.1 Plant 207, The ZSM-5 Reactor Model

A separate Fortran user block model was developed for the ZSM-5 oligomerization reactor based on the spreadsheet reactor model that was described in the Third Quarterly Report (April-June 1992). Basically this model functions as follows:

- 1. Calculates the amount of each component converted using the supplied fractional component conversions, and simultaneously accumulate the pounds of carbon, hydrogen and oxygen that have to be distributed among the products.
- 2. Distributes the carbon among the products using the supplied carbon distribution factors.

- 3. Distributes the appropriate amounts of hydrogen and oxygen among the products to maintain the component compositions.
- 4. Converts all the remaining oxygen to water.
- 5. Adjusts the hydrogen consumption to maintain a hydrogen balance.
- 6. Places the net reactor yields in the single reactor outlet stream.

In developing the ASPEN/SP model, several additional components were added to the original Fischer-Tropsch reactor loop model so that an adequate ZSM-5 reactor model could be developed. For example, C6 through C10 aromatics and naphthenes were added, the C7 through C10 paraffin/olefin pseudocomponents were split into separate paraffin and olefin components, and a C10 and heavier aromatics pseudocomponent was added.

Table 3-1 shows a comparison of the ASPEN/SP model results with those generated by the previously published spreadsheet model. For simplicity, the C7 through C10 olefin and paraffins are shown as lumped pseudo-components rather than as individual components.

The ZSM-5 oligomerization reactor model was added to the Fischer-Tropsch reactor loop model as shown in Figure 3-2. The ZSM-5 reactor model is represented by Fortran user block P207F. Block P207S is a flow splitter which acts as a two-way valve and directs the Fischer-Tropsch vapor product either through or around the ZSM-5 reactor. Block P207M is a stream mixer which mixes the streams going through and bypassing the ZSM-5 reactor. Thus, with an appropriate setting of the block P207S flow distribution parameter, this single loop model can be used to simulate both the base case and the alternate refining case.

3.2 AREA 300 PRODUCT REFINING MODEL

Simplified Fortran user block models were developed to represent all of the eight individual processing plants in Area 300 as shown in Figure 2-1. Besides doing an overall plant material balance, these models predict the utilities consumptions (productions) and the ISBL field cost for each plant. Each plant model is elementally balanced.

All Fortran user block models require four INTEGER user input parameters and up to seventy REAL user input parameters. These user input parameters control the model specific output, the prediction of the utilities consumptions (productions), and the estimation of the ISBL plant costs. In addition, some models also may require model specific user input parameters, such as the naphtha reformer model which requires the user to specify the clear Research octane number of the C5+ reformate.

For maximum flexibility and simplicity, each Fortran user block model was developed for a single inlet feed stream. In most cases, these plants have multiple inlet streams which are combined in standard ASPEN/SP mixer blocks to generate the model feed streams. Although the use of these mixer blocks enlarge the base case simulation, this technique was selected because it will simplify future modifications and enhancements to the product refining section portion of the model.

3.2.1 Plant 301, The Wax Hydrocracker

The Fortran user block model for Plant 301, the wax hydrocracker, is based on a simplified empirical yield model which requires no user supplied input parameters. This model has one inlet stream and produces five outlet streams. The single inlet stream is the mixed make-up hydrogen and Fischer-Tropsch wax streams. The five outlet streams are a C4 and lighter gas stream, a C5/C6 stream, a C7+ maphtha stream, a distillate stream, and a sour-water stream.

The make-up hydrogen rate to the Plant 301 Fortran user block model is set by an inline Fortran block named SETUP301 which sets the make-up hydrogen flow to the required rate of 1.35 wt% of the wax feed rate.

3.2.2 Plant 302, The Distiliate Hydrotreater

The Fortran user block model for Plant 302, the distillate hydrotreater, is based on a simplified empirical yield model which requires no user supplied input parameters. This model has one inlet stream and produces three outlet streams. The single inlet stream is the mixed make-up hydrogen and Fischer-Tropsch distillate streams. The three outlet streams are a C4 and lighter gas stream, a distillate product stream, and a sour-water stream.

The make-up hydrogen rate to the Plant 302 Fortran user block model is set by an inline Fortran block named SETUP302 which sets the make-up hydrogen flow to the required rate of 0.78 wt% of the distillate feed rate.

3.2.3 Plant 303, The Naphtha Hydrotreater

The Fortran user block model for Plant 303, the naphtha hydrotreater, is based on a simplified empirical yield model which requires no user supplied input parameters. This model has one inlet stream and produces four outlet streams. The single inlet stream is the mixed make-up hydrogen and Fischer-Tropsch distillate streams. The three outlet streams are a C4 and lighter gas stream, a C5/C6 stream, a C7+ naphtha stream, and a sour-water stream.

The make-up hydrogen rate to the Plant 303 Fortran user block model is set by an inline Fortran block named SETUP303 which sets the make-up hydrogen flow to the required rate of 1.48 wt% of the naphtha feed rate.

3.2.4 Plant 304, The Naphtha Reformer

The Fortran user block model for Plant 304, the naphtha reformer, is based on a simplified empirical yield model which requires one user supplied input parameter, the clear Research octane number of the C5+ reformate. The model has one inlet stream and produces three outlet streams. The single inlet stream contains the hydrocracked and hydrotreated naphthas produced by Plants 301 and 303, and the three outlet streams are a C2 and lighter gas stream, a C3/C4 gas stream, and the reformate product stream.

The single user supplied input parameter, REAL(1), is the clear Research octane number of the C5+ reformate. This simplified yield model is valid only for clear Research octane values between 88 and 101. If the user supplies a value outside of this range, a warning message will be written to the problem history file and predictions will be made for a 95 C5+ clear Research octane number, the default value.

Table 3-2 shows the simplified model output generated by the above described naphtha reformer model. This report is presented here only to show the general nature and style of each model report, and the values shown are not necessarily the final ones. For example, the plant ISBL cost has yet to be determined. Each model begins with a model specific section showing the key plant results in an easily readable form. This section is followed by a utilities section which reports the net utilities consumptions (or productions). The final section reports the plant costing information.

3.2.5 Plant 305, The C4 Isomerization Plant

The Fortran user block model for Plant 304, the C4 isomerization plant, is based on a simplified empirical yield model which requires no user supplied input parameters.

The model has one inlet stream and produces two outlet streams. The single inlet stream contains the C4s from the alkylation plant, the saturated gas plant, the purchased C4s, and a small amount of make-up hydrogen. The two product streams are a C3 and lighter gas stream and the isobutane product stream.

The make-up hydrogen rate to the Plant 305 Fortran user block model is set by an inline Fortran block named SETUP305 which sets the make-up hydrogen flow to the required rate of 0.08 wt% of the total C4 paraffin feed rate.

3.2.6 Plant 306, The C5/C6 Isomerization Plant

The Fortran user block model for Plant 306, the C5/C6 isomerization plant, is based on a simplified empirical yield model which requires no user supplied input parameters. The model has one inlet stream and produces two outlet streams. The single inlet stream contains the C5/C6 streams from the wax hydrocracking and naphtha hydrotreating plants, and a small amount of make-up hydrogen. The two product streams are a C4 and lighter gas stream and the isomerate product stream.

The make-up hydrogen rate to the Plant 306 Fortran user block model is set by an inline Fortran block named SETUP306 which sets the make-up hydrogen flow to the required rate of 0.14 wt% of the total C5/C6 paraffin feed rate.

3.2.7 Plant 307, The C3/C4/C5 Alkylation Plant

The Fortran user block model for Plant 307, the C3/C4/C5 sulfuric alkylation plant, is based on a simplified empirical yields model which requires no user supplied input parameters. The model has one inlet stream and produces four outlet streams. The single inlet stream contains the C3/C4/C5 olefins production from the Fischer-Tropsch loop and the isobutane product stream from Plant 305, the C4 isomerization plant. The four product streams are a C3 and lighter gas stream, a mostly normal C4 gas stream, the alkylate product stream, and a hydrocarbon loss stream. The hydrocarbon loss stream accounts for that hydrocarbon which is lost in the spent sulfuric acid.

3.2.8 Piant 308, The Saturated Gas Plant

The saturated gas plant takes the light hydrocarbon gas streams produced by the other seven product refining plants and produces a C2 and lighter fuel gas stream, a C3 product stream (LPG product stream), a C4 stream which goes to the C4 isomerization plant, and a sour water stream.

This plant is modeled in a different manner than the other seven product refining plants. Since no chemical reactions occur in this plant, the mass balance calculations are easily modeled by standard ASPEN/SP process blocks. A mixing block combines the seven feed streams into a single stream which is split into the four product streams by an ASPEN/SP separator block. The user supplied splitting factors determine the product stream compositions and flow rates.

F. user Fortran block located between the mixer and separator blocks predicts the utilities consumptions (or productions) and ISBL cost of the saturated gas plant.

Table 3-1 Comparison of ZSM-5 ASPEN/SP and Spreadsheet Models

	ASPEN/SIC MO	DNEE FREEFE	SPREAU HEET
OMEONENT FLOWS (LBMOL/HR)	RA-FELI	21751	MCHE
	13144	1	$1^{\circ}, 195, 2^{\circ}$
H2 N2	1238.3300	1238, 3300	1238153
*_ ([)	1387	1.087	133841.59
	52928	521-28	52028.12
002	2112.4100		
1120		2492.1165	2492.11
CIC	127: 1400	129%.5958	1299.60
(201)	386.5800	231,9480	2390
C286	96.5700	103.1839	103.19
C3H6	342.8300	205. 980	205.70
C3H8	60.3000	325.0581	325.05
1C4H8	10.3700	79.0095	79.51
SC 1H8	253.9900	152.3910	152.39
(C4H10	3.3400	380.3353	380.34
NC 1H10	63.1900	212.3039	212.30
C5H10	207.6600	201.7578	201.74
NC5H12	62.2700	154.8658	154.96
ICJH12	6.9200	311.1619	311.16
C6H12	172.0800	54.0311	54.03
NC6H14	51.6100	60.4286	60.42
1C6H14	5.7300	160.0556	160.06
C70P	189.7400	182.9039	182.92
C80P	156.9500	101.5181	101.82
C9OP	129.5900	47.3640	47.37
CIGOP	106.8000	5.2911	5.30
	87.7300	0.0	0.0
CIIOP	71.7900	0.0	C.0
CI2OP	58.4300	0.0	0.0
C130P	47.2200	0.0	0.0
CIAOP	37.8000	0.0	0.0
C150P	29.9000	0.0	0.0
C160P		0.0	0.0
C170P	23.3300	0.0	0.0
CIBOP	17.9400		
C190P	13.0400	0.0	0.0
WAX	3.0100	0.0	0.0
OXVAP	42.9500	0.0	0.0
OXHC	158.1200	0.0	0.0
OXH2O	157.4000	0.0	0.0
C5N	0.0	7.9367	7.91
C6N	C.O	37.4750	37.18
C7N	0.0	39.6837	39.68
CBN	0.0	34.7232	34.72
Can	0.0	11.7581	11.76
CION	0.0	1.3227	1.32
C6A	0. 0	21.2511	21.25
C7A	0.0	83.1468	83.15
C8A	0.0	112 2000	142.20
C9A	0. 0	104.3535	104.35
CIDAP	0.0	<u> </u>	72.10
τοτλί	90197	91370	913 73.70

Table 3-2

Sample Model Sumary Report for The Naphtha Reforming PLant

COMPONENT FLOW RAT				
COMPONENT		12- GASES	0.5018	REFORMATE
112	.000	4.282	-	.000
1120	.000	.000		.000
CH1	.000	1.125	.000	.000
C2116	.000	3.053	.000	
1 3118	.000	.000	3.282	.000
103110	.000	.000	2.334	.000
NC 1H10	.000	.000	2,901	.000
NC5H12	.000	.000	.000	.000
IC5H12	.000	.000	.000	.000
NC6H14	.000	.000	.000	.000
106H14	.000	.000	.000	.000
C7-300HC	41.074	.000	. 000	.000
3-350HC	13.190	.000	.000	.000
C7-300HT	54.634	- 000	. 000	.000
3-350HT	15.519	.000	.000	
REFORMAT	.000	.000	.000	
OTHERS	.000	.000		
TOTAL	124.417	8.460	9.120	106.837
CJ+ RONC CJ+ (R+M)/2 C5+ SG RVP, PSI BENZENE, WTX AROMATICS, WTX				95.0 90.0 .7724 3.4 .7 65.9
	100.0	100.0	120.0	130.0
TEMPERATURE, F PRESSURE, PSIA		50.0		
PLANT UTILITIES CO POWER, KW 900 PSIG/1000 F S 360 PSIG/440 F ST 600 PSIG/720 F ST 600 PSIG SATD STE 150 PSIG SATD STEA 9LANT FUEL, MM BT COOLING WATER, MG PROCESS WATER, MG NITROGEN, MM SCF/	TEAM, MLBS/HR EAM, MLBS/HR AM, MLBS/HR AM, MLBS/HR AM, MLBS/HR M, MLBS/HR US/HR AL/HR AL/HR		2933. .0 .0 -21.7 .0 .3 .0 108.50 44.84 .00 .00	
TOTAL PLANT OPERA	TORS/DAY		10.0	

PLANT COSTING INFORMATION

TOTAL NUMBER OF DUPLICATE TRAINS	1
MAXIMUN SIZE, MLBS/HR	150.000
MINIMUM SIZE, MLBS/HR	1.000
CAPACITY, MLBS/IIR	124.417
PLANT ISBL FIELD COST, MMS	20.000

Baseline Study F-T

Figure 3-1 ASPEN/SP Model Flow Diagram for Area 200 - Fischer-Tropsch Loop

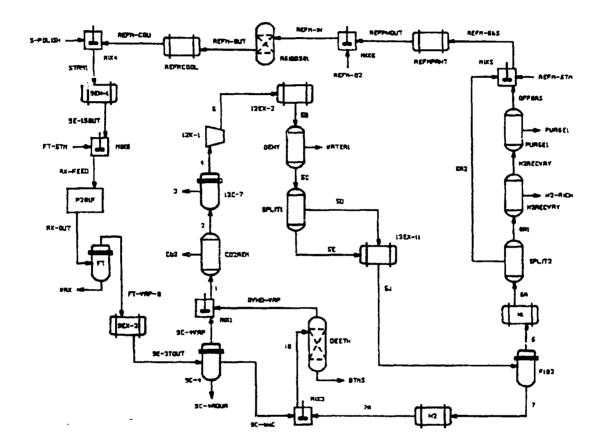
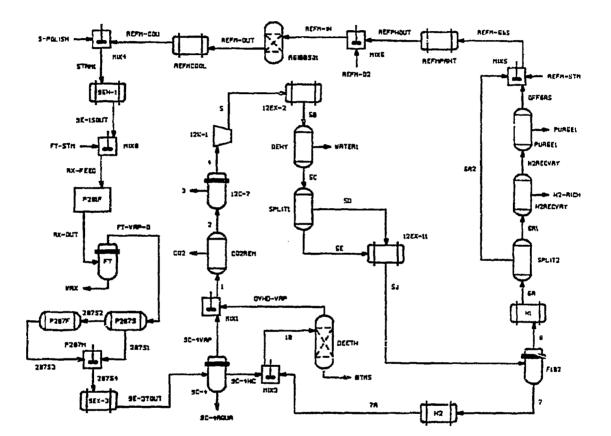


Figure 3-2 ASPEN/SP Model Flow Diagram for Area 200 with ZSM-5 Reactor



Project Management & Staffing Report

4.1 TASK 7 - PROJECT MANAGEMENT

During this reporting period, a project progress meeting was held at Bechtel San Francisco office. Details of the Baseline and the two Alternate Cases' designs and their progresses were reviewed.

4.2 KEY PERSONNEL STAFFING REPORT

The key personnel staffing report for this reporting period as required by DOE/PETC is shown below:

Name	Function	% Time Spent ^(a)
Bechtel		
Yang L. Cheng	Process Supervisor	75
Charles R. Brown	Offsite Facilities	0 (b)
Gary Lucido	Cost Estimating	0(c)
Samuel S. Tam	Project Manager	31
Gerald N. Choi	Process Engineer	70
Amoco		
A. Schachtschneider	Subcontract Manager	2
S. S. Kramer	Process Model/Simulation	75

(a) Number of hours spent divided by the total available working hours in the period and expressed as a percentage.

(b) C. Brown of Bechtel did not spend any time in this reporting quarter because no offsite facilities work was required.

(c) G. Lucido of Bechtel did not spend any time in this reporting quarter because no cost estimating work was required.

Figure 4-1

Overall Milestone Schedule

(as of March 14, 1993)

TTLE Baseline Design/Economics for Advanced 2.REPORTING PERIOD Fischer-Tropsch Technology 2/15/93 10 3/15/93			J IDENTIFICATION NUMBER DE AC22-91PC90	J IDENTIFICATION NUMBER DE 4C22-91PC90C2"			
		Bechlei Corporation 50 Beale Street San Francisco, CA 94105	5 START DATE 92691 6 COMPLETION DATE 92593				
ELEMENT	REPORTING ELEMENT	ROTRATION FY 92 O N: D JI F M A M J J A S O N		·: 020:00 • • • • • •			
Task 1	Basenne Design	0 0	/	99' 96			
Task 2	Economic Evaluation			82 23			
Task 3	Engineering Design Chiena	in the second		35			
Tasa 4	Process Flowsheet Simulation Model	taith taitaite in 18-		69 32			
Task 5	Sensitivity Studies						
Tasx 6	Documentation and Training			<u> </u>			
Task 7	Project Management & Administration						
ୗଡ଼ଡ଼ଡ଼	Completion ASPEN/SP software delivered First progress meeting Second progress meeting	Baseline case design complete Baseline case equipment list transmitted to Cost E	simating				
IT SCHATU	I	NC DATE Samuel S. Tam	Q 5/27/93				

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