BASELINE DESIGN/ECONOMICS FOR ADVANCED FISCHER-TROPSCH TECHNOLOGY. QUARTERLY REPORT, JULY--SEPTEMBER 1993

DEPARTMENT OF ENERGY, PITTSBURGH, PA.
PITTSBURGH ENERGY TECHNOLOGY CENTER

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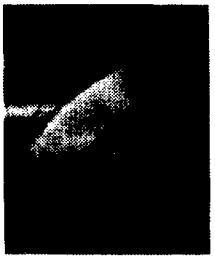

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Baseline Design/Economics for Advanced Fischer-Tropsch Technology

Contract No. DE-AC22-91PC90027

Quarterly Report

July – September 1993

U.S. Department of Energy
Pittsburgh Energy Technology Center

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Section 1

Introduction and Summary

This report is Bechtel's eighth quarterly technical progress report and covers the period of July through September, 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.

- 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.

- 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:

- Task 1: Establish the baseline design and alternatives.

- Task 2: Evaluate baseline and alternative economics.

- Task 3: Develop engineering design criteria.

- Task 4: Develop a process flowsheet simulation (PFS) model.

- 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.

During the period of this report, a Topical Report summarizing the Baseline Case design was drafted and issued to DOE/PETC for review and release approval. Major effort was spent on the Alternate Upgrading and Refining Case. Its design specifications were finalized, and material and utility balances completed. Initial capital cost estimates were developed. A Topical Report, summarizing the Alternative (ZSM-5) Upgrading and Refining Case design, is being drafted.

Under Task 4, some of the individual plant models were expanded and enhanced. An overall ASPEN/SP process simulation model was developed for the Baseline Design Case by combining the individual models of Areas 100, 200 and 300. In addition, a separate model for the simplified product refining area, Area 300, of the Alternate Upgrading and Refining case was developed.

Under Task 7, cost and schedule control was the primary activity. A technical paper entitled "Baseline Design/Economics for Advanced Fischer-Tropsch Technology" was presented in the DOE/PETC's Annual Contractors Review Conference, held at Pittsburgh, Pennsylvania, on September 27-29, 1993. A contract amendment was submitted to include the Kerr McGee ROSE unit in the Baseline design case and to convert the PFS models from the ASPEN/SP to ASPEN/Plus software code.

Section 2

Task 1 - Alternate (ZSM-5) Refining Case

Work progressed during this quarter consists mainly of 1) finished drafting of a Topical Report which summarizes the Baseline Case design, and issued it to DOE/PETC for review and release approval; 2) completed the design specifications, material and utility balances for the Alternative Upgrading & Refining case using ZSM-5. Initial capital cost estimates were also developed. A Topical Report, summarizing the Alternative (ZSM-5) Upgrading & Refining design, is being drafted.

2.1 DESIGN BASIS AND SPECIFIC CONSIDERATIONS

The design basis for the Illinois No. 6 Coal Alternative Upgrading case with ZSM-5 is almost identical to that of the Baseline case design. The inclusion of a fixed-bed ZSM-5 reactor into the F-T Synthesis Loop is to duplicate the two-stage process piloted by Mobil. The ZSM-5 step radically alters the character of the F-T naphtha and light distillate fractions by converting 1-olefins and paraffins above C_7 and oxygenates into isoparaffins, isoolefins, naphthenes and aromatics. This results in a higher ratio of naphtha to distillate products. Wax hydrocracking, alkylation and light ends recovery are still required, but no further processing of the naphtha and distillate products is needed.

The design of the plants in Area 100, Syngas Preparation, remains identical to that of the Baseline design. Only the plants in the F-T synthesis loop (Area 200) and downstream processing of Area 300 are impacted. Many of the these plants, however, can be prorated from the Baseline study.

Primary differences in design from the Baseline design are as follows:

1. Inclusion of ZSM-5 reactors into the F-T Synthesis Loop. Nine trains of ZSM-5 reactors are provided, eight in operation and one in regeneration mode, to handle all the effluents from the 24 F-T reactors. Design of the ZSM-5 reactor is based on Mobil's pilot plant work and it was discussed in some details in the April-June 1992 Quarterly Report.

2. As a result of generating a more upgraded product, Catalytic Reforming, C5/C6 Isomerization, Naphtha and Distillate Hydrotreating plants are eliminated from Area 300.

3. Oxygenate wash towers are eliminated from Plants 201 and 204, since the ZSM-5 converts all the oxygenates in the vapor stream into hydrocarbons.

2.2 BLOCK FLOW DIAGRAM

Alternate (ZSM-5) Upgrading & Refining Case block flow diagrams for Area 100A (Syngas Production), Area 200A (F-T Synthesis/ZSM-5 Reaction), and Area 300A (Upgrading and Refining) are shown in Figure 2-1 to 2-3 respectively. The suffix "A" was included to designate alternate upgrading. These block flow diagrams show the major process interconnections between the various primary plants.

The Area 100A and 200A block flow diagrams are essentially identical to those of the Baseline Case. The only difference is the inclusion of the ZSM-5 step in Plant 201. This, of course, has an effect on the material balance in Area 200A. The Area 300A block flow diagram represents a considerable simplification over the Baseline design.

2.3 DETAILED PROCESS FLOW DIAGRAM

The Area 100A PFDs are identical to those of the Baseline Case. The Area 200A PFDs are included in this Quarterly.

2.4 F-T SYNTHESIS/ZSM-5 PROCESS DESCRIPTION

The only major differences in design between the Illinois No. 6 Coal Alternative Upgrading and the Baseline Study are: (1) the inclusion of ZSM-5 reactors with ZSM-5 catalyst regeneration into the F-T Synthesis Loop, and the elimination of downstream oxygenate wash towers from Area 200, and (2) the elimination of several catalytic upgrading processing Plants (i.e., Catalytic Reforming, C5/C6 Isomerization, Naphtha and Distillate Hydrotreating) from Area 300. Area 100 is essentially identical to that of the Baseline study.

2.4.1 Plant 201A - F-T Synthesis And ZSM-5 Reaction

The principle function of this plant is to convert syngas from Area 100 into hydrocarbon products using slurry phase Fischer-Tropsch and fixed bed ZSM-5 reactors. Since the syngas conversion per pass is 82.0%, Plant 201 is part of an overall recycle synthesis loop which is called Area 200.

The Alternate Case differs from the Baseline Design due to the inclusion of ZSM-5 reactors downstream of the Fischer-Tropsch reactors. The primary purpose of the ZSM-5 reactors is to increase the overall liquid product yield by converting the F-T reaction vapors to a high quality gasoline. Specifically, olefins, oxygenates and

heavy paraffins in the F-T vapor are converted into a mixture of isoparaffins, iso-olefins, naphthenes and aromatics.

Design Basis and Considerations

A total of 24 operating F-T 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. Nine trains of ZSM-5 reactors are provided, eight in operation and one in regeneration mode. Although a smaller number of ZSM-5 reactors was feasible, eight was chosen to match the number of trains and to reduce complexity.

A total of 8 process equipment trains are needed downstream of the F-T and ZSM-5 reactors to process the 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.

F-T Reaction

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 488 °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 H_2/CO inlet ratio (0.361 in the Area 100 syngas and 0.456 at the reactor inlet) and water vapor addition rate, the yield model shows that CO conversion is 87.2 % and overall H_2 + CO conversion is 82.0 mole%. A total of 5998 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 6.9%. This water compensates for the low H_2/CO ratio by promoting additional H_2 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.

ZSM-5 Reaction

Mobil's pilot plant data was again utilized to develop the design correlations for predicting overall product distribution. The Mobil data provided component breakdowns for both the feed and products for two different types of feedstock. The first type was the F-T vapor from a low wax F-T run. The second type was the F-T vapor from a high wax run. The ZSM-5 component conversion factors for each feedstock were calculated and averaged. An atom balance was used to balance the flows between feed and product.

An analysis of the Mobil data shows that there is a definite pattern in the conversion and yield in both the high and low wax yield cases:

- A large portion of the 1-olefins and of the paraffins above C_7 are converted along with all of the oxygenates
- Isoparaffins, isoolefins, naphthenes and aromatics are formed
- There is no conversion of H_2, CO, CO_2 or H_2O
- All of the oxygen atoms from the oxygenates end up as H_2O

The reactor size was based on having eight reactors in operation and using approximately the same space velocity and superficial velocity as were used in the Mobil pilot plant work.

2.4.2 Process Description (PFD 201-B-01, 02, 03, 04)

The process flow diagrams for Plant 201, F-T Synthesis, are shown in PFD 201-B-01 through PFD 201-B-04.

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 352 °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 non-vaporizable 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. The vapors from 201C-9 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, 201C-5, 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 6 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 based on current knowledge of the catalyst system, its characteristics and commercial separation equipment available. Extensive pilot plant work and engineering is required to confirm the validity of the assumptions made in the development of this separation scheme.

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. On PFD 201-B-04, the vapor stream at 488 °F and 289 psig is routed to the ZSM-5 feed/product exchanger, 201E-8, where the vapor is heated up to the ZSM-5 reactor inlet temperature (572°F at start of run conditions). The ZSM-5 reaction is exothermic and there is a 72 °F rise across the reactor, 201C-16. After heating up the feed, the reactor effluent is sent to a steam generator, 201E-9, where low pressure steam is made. The effluent is further 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, where the aqueous water stream, the liquid hydrocarbons stream, and the vapor stream are separated.

The ZSM-5 system is supplied with a single startup fired heater, 201F-2, which can be used for any of the nine ZSM-5 trains. A single regeneration system is supplied for the entire plant. Regeneration consists of heating up an air/nitrogen stream through heat exchange in 201E-10 and fired heating in 201F-3. (Nitrogen is used to limit the temperature across the reactor bed.) This stream is used to burn off coke that has laid down on the reactor catalyst. The vent gases from 201E-10 are cooled further in 201E-11 and 201E-12 prior to being sent to separator 201C-17 where water is removed. The overhead is split into a purge stream which is sent to the flare and a recycle stream which is sent to the regeneration gas compressor, 201K-3. The discharge gases are then mixed with air from compressor 201K-2.

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 CO_2 recovery plant, Plant 202.

It is estimated that about 6 TPD of makeup catalyst (0.5% of the catalyst inventory per day) is required to maintain the catalyst inventory level in the F-T reactors. This corresponds to an expected catalyst life of 200 days. 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.

2.5 MATERIAL BALANCE SUMMARY

The overall material balance for the Alternate Upgrading and Refining Case is shown in Tables 2-1 to 2-7, for Areas 200A and 300A. These are presented in sequential order in accordance with the major process area and plant numbers. Detailed component material balances are given for each major streams leaving and entering a plant. Streams are identified with a stream number identical to that which appears in the PFDs.

Table 2-1

Material Balance Summary
Plant 201A-Fischer Tropsch Synthesis/ZSM5 Reaction
(Illinois No. 6 Coal Alternative Upgrading)

Stream No.	201.1	201.2	201.3	201.4	201.5	201.6	201.7
	Syngas from sulfur Polishing	Water addition To FT	Feed To F-T Reactor	F-T Vapor/ ZSM5 Feed	Wax	Produced H2O To WW Treatment	Off Gas To Fuel
Phase	Vap	Liq	Vap	Vap	Liq	Liq	Vap
Component Flows LBmol/hr							
H2	33,269.00		45,746.00	13,501.00	0.60	0.00	3.15
N2	965.05		3,207.66	3,206.81	0.13		0.72
O2							
CO	92,241.00		100,380.00	12,855.00	0.56	0.00	2.97
CO2	3,819.53		5,809.79	53,893.00	10.26	3.26	23.31
H2O	472.76	5,997.54	11,452.00	2,239.80	3.02	2,213.60	1.69
CH4	22.77		411.16	1,363.49	0.13	0.00	0.45
C2H4			0.01	389.33	0.09		0.18
C2H6			0.01	97.33	0.03		0.05
C3H6				345.26	0.19		0.22
C3H8				60.92	0.04		0.04
IC4H8				13.47	0.02		0.01
NC4H8				255.78	0.29		0.19
IC4H10				3.36	0.00		0.00
NC4H10				63.94	0.08		0.05
C5H10				209.13	0.40		0.16
IC5H12				6.97	0.01		0.01
NC5H12				62.71	0.15		0.05
C6H12				173.31	0.66		0.11
IC6H14				5.78	0.02		0.00
NC6H14				51.97	0.22		0.03
C7-C10 OP				977.15	52.24		0.12
C5-C10 AN							
WAX				3.05	453.93		
OXVAP				43.12	0.10		0.03
OXHC				163.62	1.46		0.02
OXH2O				158.05	0.36		0.09
Catalyst							
Total	130,820.12	5,997.54	167,006.63	90,143.36	524.98	2,216.87	33.65
Total lb/hr	2,854,800	108,050	3,462,200	3,168,800	292,180	40,022	1,253
Mol. Wt.	21.82	18.02	20.73	35.15	556.55	18.05	37.24
MMSCFD	1,191.51		1,521.10	821.03			

Table 2-1 (Cont.)

Material Balance Summary
Plant 201A-Fischer Tropsch Synthesis/ZSM5 Reaction
(Illinois No. 6 Coal Alternative Upgrading)

Stream No.	201.10	201.11	201.12	201.13	201.14
	HC Liquid	Unconverted Syngas	Pretreated Catalyst To F-T	Waste Catalyst To Disposal	ZSM5 Product Stream
Phase	Liq	vap	Slurry	Solid	Vap
Component Flows LBmol/hr					
H2	2.90	13,393.00			13396.00
N2	1.06	3,205.74			3206.81
O2					
CO	4.66	12,850.00			12855.00
CO2	230.01	53,659.00			53893.00
H2O	42.40	388.88			2624.82
CH4	1.42	1,388.68			1390.10
C2H4	0.87	232.73			233.60
C2H6	0.56	103.43			103.98
C3H6	3.05	204.10			207.15
C3H8	5.42	321.61			327.03
IC4H8	3.35	76.64			80.00
NC4H8	6.59	146.88			153.47
IC4H10	13.47	369.11			382.57
NC4H10	10.49	203.14			213.62
C5H10	22.13	180.84			202.97
IC5H12	32.72	280.27			312.99
NC5H12	20.51	135.35			155.85
C6H12	14.54	39.83			54.37
IC6H14	38.30	122.71			161.01
NC6H14	17.90	42.94			60.84
C7-C19 OP	220.62	118.94			339.56
C5-C10 AN	430.62	131.66			562.29
WAX			1652.25*	24.25*	
OXVAP					
OXHC					
OXH2O					
Catalyst			479.75*	479.75*	
Total	1,123.58	87,575.49			90,917.04
Total lb/hr	98,198	3,030,600	2132	504	3,168,800
Mol. Wt.	87.40	34.61			34.85
MMSCFD		797.64			828.07

Table 2-2

Material Balance Summary
Plant 202A-CO2 Removal
(Illinois No. 6 Coal Alternative Upgrading)

Stream No.	202.1	202.2	202.3	202.4
	Unconverted Syngas From F-T	Deethanizer Overhead Vapor	Recycle Gas To Compressor	Scrubbed CO2
Phase	Vap	Vap	Vap	Vap
Component Flows Lbmol/hr				
H2	13,393.00	25.27	13,418.00	
N2	3,205.74	32.46	3,238.14	
O2				
CO	12,850.00	157.76	13,008.00	
CO2	53,659.00	413.52	270.36	53,802.00
H2O	368.88		368.87	
CH4	1,388.68	95.35	1,484.04	
C2H4	232.73	244.96	477.71	
C2H6	103.43	204.08	307.52	
C3H6	204.10	10.41	214.51	
C3H8	321.61	9.76	331.38	
IC4H8	76.64		76.64	
NC4H8	146.88		146.88	
IC4H10	369.11		369.10	
NC4H10	203.14		203.14	
C5H10	180.84		180.84	
IC5H12	280.27		280.26	
NC5H12	135.35		135.34	
C6H12	39.83		39.83	
IC6H14	122.71		122.71	
NC6H14	42.94		42.94	
C7-C19 OP	118.94		118.94	
C5-C10 AN	131.66		131.66	
WAX				
OXVAP				
OXHC				
OXH2O				
Total	87,575.49	1,193.57	34,966.82	53,802.00
Total lb/hr	3,030,600	38,985	701,710	2,367,800
Mol.Wt	34.61	32.66	20.07	44.01
MMSCFD	797.64	10.87	318.48	490.03

Table 2-3

Material Balance Summary
Plant 203A-Compression & Dehydration
(Illinois No. 6 Coal Alternative Upgrading)

Stream No.	203.1	203.2	203.3	203.4	203.5	203.6	203.7
	Syngas From CO2 Removal	Liquid Hydrocarbons To Deethanizer	Syngas To Hydrocarbons Recovery	Water To Waste Treatment	Unused Fuel Gas From H2 Recovery	Fuel Gas From H2 Recovery/ Regeneration	Total Fuel Gas To Gas Header
Phase	Vap	Liq	Vap	Liq	Vap	Vap	Vap
Component Flows LBmol/hr							
H2	13,418.00	1.97	13,416.00		896.28	1130.58	2026.86
N2	3,238.14	0.74	3,237.41		428.28	540.24	968.52
O2							
CO	13,008.00	3.24	13,004.00		1,716.80	2165.61	3882.41
CO2	270.36	0.80	269.57		11.27	14.21	25.48
H2O	388.87	28.61		254.64			87.62
CH4	1,484.04	1.05	1,483.00		185.66	234.19	419.85
C2H4	477.71	1.25	476.46		31.07	39.19	70.26
C2H6	307.52	1.17	306.36		12.52	15.79	28.30
C3H6	214.51	2.29	212.22		1.26	1.59	2.84
C3H8	331.38	4.03	327.34		1.52	1.91	3.43
IC4H8	76.64	2.43	74.21		0.04	0.06	0.10
NC4H8	146.88	4.76	142.12		0.08	0.10	0.19
IC4H10	369.10	9.90	359.21		0.33	0.42	0.76
NC4H10	203.14	7.62	195.52		0.08	0.11	0.19
C5H10	180.84	15.33	165.50		0.01	0.01	0.02
IC5H12	280.26	23.37	256.89				0.04
NC5H12	135.34	14.34	121.00		0.00	0.01	0.01
C6H12	39.83	9.02	30.81				0.00
IC6H14	122.71	24.75	97.96				0.00
NC6H14	42.94	10.89	32.05				0.00
C7-C19 OP	118.94	66.46	52.48				
C5-C10 AN	131.66	72.30	59.37				
WAX							
OXVAP							
OXHC							
OXH2O							
Total	34,966.82	304.30	34,319.48	254.64	3,285.20	4,144.02	7,516.88
Total lb/hr	701,710	24,294	671,250	4,587	66,768	84,222	152,568
Mol. Wt.	20.07	79.83	19.56	18.02	20.32	20.32	20.30
MMSCFD	318.48		312.58		29.92	37.74	68.46

Table 2-4

Material Balance Summary
Plant 204A-Hydrocarbon Recovery
(Illinois No. 6 Coal Alternative Upgrading)

Stream No.	204.1	204.2	204.3	204.4	204.5	204.6	204.7
	Syngas To H2 Recovery	Syngas From Dehydration	HC Liquids To Deethanizer	HC Liquids From Compr & Dehy	HC Liquids From F-T Reactor	Deethanizer Underflow	Deethanizer Overhead Vapor
Phase	vap	Vap	Liq	Liq	Liq	Liq	Vap
Component Flow Lbmol/hr							
H2	13,396.00	13,416.00	20.40	1.97	2.90		25.27
N2	3,206.75	3,237.41	30.66	0.74	1.06		32.46
O2							
CO	12,855.00	13,004.00	149.85	3.24	4.66		157.76
CO2	84.36	269.57	185.21	0.80	230.01	2.50	413.52
H2O				26.61	42.40	69.01	
CH4	1,390.11	1,483.00	92.89	1.05	1.42		95.35
C2H4	232.63	476.46	243.83	1.25	0.87	0.98	244.96
C2H6	93.71	306.36	212.65	1.17	0.56	10.29	204.08
C3H6	9.41	212.22	202.81	2.29	3.05	197.74	10.41
C3H8	11.36	327.34	315.99	4.03	5.42	315.67	9.76
IC4H8	0.33	74.21	73.88	2.43	3.35	79.66	
NC4H8	0.62	142.12	141.50	4.76	6.59	152.85	
IC4H10	2.50	359.21	356.71	9.90	13.47	380.07	
NC4H10	0.83	195.52	194.89	7.62	10.49	213.00	
C5H10	0.07	165.50	165.43	15.33	22.13	202.89	
IC5H12	0.14	256.89	256.76	23.37	32.72	312.84	
NC5H12	0.03	121.00	120.97	14.34	20.61	155.81	
C6H12	0.00	30.81	30.81	9.02	14.54	54.37	
IC6H14	0.01	97.96	97.95	24.75	38.30	161.00	
NC6H14	0.00	32.05	32.05	10.89	17.90	60.84	
C7-C19 OP		52.48	52.48	66.46	220.62	339.56	
C5-C10 AN		59.37	59.36	72.30	430.62	562.28	
WAX							
OXVAP							
OXHC							
OXH2O							
Total	31,283.65	34,319.48	3,037.07	304.30	1,123.58	3,271.39	1,193.57
Total lb/hr	513,400	671,250	157,850	24,294	98,198	241,360	38,985
Mol. Wt.	16.41	19.56	51.97	79.83	87.40	73.78	32.66
MMSCFD	284.93	312.58					10.87

Table 2-4 (Cont.)
Material Balance Summary
Plant 204A-Hydrocarbon Recovery
(Illinois No. 6 Coal Alternative Upgrading

Stream No.	204.12	204.13	204.15	204.19
	Feed To Product Fractionator	Fractionator Overhead To Alkylation	Naphtha To Gasoline Pool	Wax To Hydrocracking Plant
Phase	Liq	Vap	Vap/Liq	Liq
Component Flows Lbmol/hr				
H2	0.60			
N2	0.13			
O2				
CO	0.66			
CO2	12.75			
H2O	72.04			
CH4	0.13			
C2H4	1.07			
C2H6	10.32			
C3H6	197.94	197.94		
C3H8	315.71	315.71		
IC4H8	79.68	79.68		
NC4H8	153.14	153.14		
IC4H10	380.07	380.07		
NC4H10	213.08	213.08		
C5H10	203.29	203.29		
IC5H12	312.86	312.86		
NC5H12	155.96	155.96		
C6H12	55.03		55.03	
IC6H14	161.02		61.06	
NC6H14	61.06		161.02	
C7-C19 OP	391.80		346.52	45.28
C5-C10 AN	562.28		562.28	
WAX	453.93			453.93
OXVAP	0.10			
OXHC	1.46			1.46
OXH2O	0.36			
Total	3,796.38	2,011.74	1,186.92	500.67
Total lb/hr	533,540	117,870	122,800	290,620
Mol. Wt.	140.54	58.59	103.55	580.46
MMSCFD		18.32		

Table 2-5

Material Balance Summary
Plant 205A-Hydrogen Recovery
(Illinois No. 6 Coal Alternative Upgrading)

Stream No.	205.2	205.3	205.4	205.5
	Recycle Gas From Plant 204	H2 Product From PSA	Fuel (Purge) Gas	Autothermal Reformer Feed
Phase	Vap	Vap	Vap	Vap
Component Flows Lbmol/hr				
H2	13,396.00	2,019.06	2026.86	9,350.02
N2	3,206.75		968.52	2,238.23
C2				
CO	12,855.00		3882.41	8,972.16
CO2	84.36		25.48	58.88
H2O				
CH4	1,390.11		419.85	970.26
C2H4	232.63		70.26	162.37
C2H6	93.71		28.30	65.41
C3H6	9.41		2.84	6.57
C3H8	11.36		3.43	7.93
IC4H8	0.33		0.10	0.23
NC4H8	0.62		0.19	0.43
IC4H10	2.50		0.76	1.74
NC4H10	0.63		0.19	0.44
C5H10	0.07		0.02	0.05
IC5H12	0.14		0.04	0.10
NC5H12	0.03		0.01	0.02
C6H12	0.00		0.00	0.00
IC6H14	0.01		0.00	0.00
NC6H14	0.00		0.00	0.00
C7-C19				
C5-C10 AN				
WAX				
OXVAP				
OXHC				
OXH2O				
Total	31,283.65	2,019.06	7,429.26	21,834.84
Total lb/hr	531,400	4,070	150,990	358,340
Mol. Wt.	16.99	2.02	20.32	16.41
MMSCFD	284.93	18.39	67.67	198.87

Table 2-6

Material Balance Summary
Plant 206A-Autothermal Reformer
(Illinois No. 6 Coal Alternative Upgrading)

Stream No.	206.1	206.2	206.3	206.4
	Oxygen Addition To Reformer	Steam Addition To Reformer	Syngas From H2 Recovery	Recycle Gas To F-T Reactor
Phase	Vap	Vap	Vap	Vap
Component Flows Lbmol/hr				
H2			9,350.02	12,447.00
N2	4.39		2,238.23	2,242.62
O2	838.97			
CO			8,972.16	8,133.92
CO2			58.88	1,990.25
H2O		6,328.57		4,982.01
CH4			970.26	388.38
C2H4			162.37	0.01
C2H6			65.41	0.01
C3H6			6.57	
C3H8			7.93	
IC4H8			0.23	
NC4H8			0.43	
IC4H10			1.74	
NC4H10			0.44	
C5H10			0.05	
IC5H12			0.10	
NC5H12			0.02	
C6H12			0.00	
IC6H14			0.00	
NC6H14			0.00	
C7-C19 OP				
C5-C10 AN				
WAX				
OXVAP				
OXHC				
OXH2O				
Total	843.36	6,328.57	21,834.84	30,184.21
Total lb/hr	26,969	114,010	358,340	499,320
Mol. Wt.	31.98	18.02	16.41	16.54
MMSCFD	7.68	57.64	198.87	274.92

Table 2-7 (1)

Area 300A -Product Upgrading and Refining
Material Balance Summary

	<----------		Wax Hydrocracking			---------->		<----------	
	Feed	H2 Required	Produced	Produced	Produced	Produced	Produced	Olefin Feed	iC4 Makeup
Component			C4-	C5/C6's	C7+ Naphtha	Distillate	H2O		
H2		3923	0	0	0	0		0	0
N2	0		0	0	0	0		0	0
CO	0		0	0	0	0		0	0
CO2	0		0	0	0	0		0	0
H2O	0		0	0	0	0		0	0
C1	0		144	0	0	0		0	0
C2=	0		0	0	0	0		0	0
C2	0		144	0	0	0		0	0
C3=	0			0	0	0		8329	0
C3	0		4273	0	0	0		13922	0
IC4	0		5659	0	0	0		22091	14725
nC4	0		4591	0	0	0		12385	483
C4=	0		0	0	0	0		13063	0
iC5	0		0	7045	0	0		22573	0
nC5	0		0	5948	0	0		11253	0
C5=	0		0		0	0		14258	0
C6=	0		0	0	0	0		0	0
iC6	0		0	11203	0	0		0	0
nC6	0		0	6872	0	0		0	0
C7-C10 (Naphtha)	0		0	0	0	0		0	0
C11-C19 (Distillate)	10047		0	0	0	0		0	0
C19+ (Wax)	280450		0	0	0	0		0	0
180-300OX	92		0	0	0	0		0	0
300-350OX	5		0	0	0	0		0	0
350-700OX	29		0	0	0	0		0	0
Reformate	0		0	0	0	0		0	0
C3 Alkylate	0		0	0	0	0		0	0
C4 Alkylate	0		0	0	0	0		0	0
C5 Alkylate	0		0	0	0	0		0	0
C5 Isomerate	0		0	0	0	0		0	0
C6 Isomerate	0		0	0	0	0		0	0
C7-300 HC	0		0	0	41808	0		0	0
300-350 HC	0		0	0	13428	0		0	0
350-500 HC	0		0	0	0	61211		0	0
500-700 HC	0		0	0	0	130300		0	0
C7-300 HTU	0		0	0	0	0		0	0
300-350 HTU	0		0	0	0	0		0	0
350-500 HTU	0		0	0	0	0		0	0
500+ HTU	0		0	0	0	0		0	0
C5-C10 AN									
H2O Produced	0		0	0	0	0	1918	0	0
Total (Lb/hr)	*290623*	*3923*	*14811*	*31068*	*55234*	*191511*	*1918*	*117874*	*15208*
Total (BPSD)							*132*		
Density (lb/ft3)							*62.2978*		
Mol. Wt	*580.46*	*2.02*	*51.60*	*79.70*	*134.11*	*234.34*	*18.02*	*68.59*	*58.12*

Table 2-7 (2)

Area 300A -Product Upgrading and Refining
Material Balance Summary

	C3/C4/C5 Alkylation				C4 Isomerization			Saturated	
	Produced	Produced	Produced	HC Acid Loss	Feed	H2 Required	Produced	C4'S	C2- Fuel Gas
Component	C4's	Alkyates	C3-				Fuel gas		
H2	0	0	0		0	6	0	0	1
N2	0	0	0		0		0	0	4
CO	0	0	0		0		0	0	16
CO2	0	0	0		0		0	0	561
H2O	0	0	0		0		0	0	0
C1	0	0	0		0		23	0	170
C2=	0	0	0		0		0	0	0
C2	0	0	0		0		52	0	496
C3=	0	0	0		0		0	0	0
C3	0	0	13922		0		140	0	0
IC4	0	0	0		5546		0	0	0
nC4	12868	0	0		9872		0	7495	0
C4=	0	0	0		0		0	0	0
iC5	0	22573	0				0	0	0
nC5	0	11253	0		0		0	0	0
C5=	0	0	0		0		0	0	0
C6=	0	0	0		0		0	0	0
iC6	0	0	0		0		0	0	0
nC6	0	0	0		0		0	0	0
C7-C10 (Naphtha)	0	0	0		0		0	0	0
C11-C19 (Distillate)	0	0	0		0		0	0	0
C19+ (Wax)	0	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	0	0	0		0		0	0	0
C3 Alkylate	0	25815	0		0		0	0	0
C4 Alkylate	0	25098	0		0		0	0	0
C5 Alkylate	0	20798	0		0		0	0	0
C5 Isomerate	0	0	0		0		0	0	0
C6 Isomerate	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		0	0	0
500-700 HC	0	0	0		0		0	0	0
C7-300 HTU	0	0	0		0		0	0	0
300-350 HTU	0	0	0		0		0	0	0
350-500 HTU	0	0	0		0		0	0	0
500+ HTU	0	0	0		0		0	0	0
C5-C10 AN									
H2O Produced	0	0	0	757	0		0	0	0
Total (Lb/hr)	*12868*	*105535*	*13922*	*757*	*15418*	*6*	*215*	*7495*	*1248*
Total (BPSD)								*862*	
Density (lb/ft3)							*31.7323*		
Mol. Wt	*58.12*	*96.24*	*44.10*	*114.23*	*58.12*	*2.02*	*33.92*	*58.12*	*30.35*

Table 2-7 (3)

Area 300A -Product Upgrading and Refining
Material Balance Summary

	Gas plant/Product Recovery			
	C3	H20	Gasoline	Diesel
Component				
H2	0		0	0
N2	0		0	0
CO	0		0	0
CO2	0		0	0
H2O	0	1298	0	0
C1	0		0	0
C2=	30		0	0
C2	10		0	0
C3=	0		0	0
C3	16036		0	0
IC4	113		0	0
nC4	92		0	0
C4=	0		0	0
IC5	0		29618	0
nC5	0		17200	0
C5=	0		0	0
C6=	0		4631	0
IC6	0		25079	0
nC6	0		12134	0
C7-C10 (Naphtha)	0		37606	0
C11-C19 (Distillate)	0		0	0
C19+ (Wax)	0		0	0
150-300OX	0		0	0
300-350OX	0		0	0
350-700OX	0		0	0
Reformate	0		0	0
C3 Alkylate	0		25815	0
C4 Alkylate	0		26098	0
C5 Alkylate	0		20796	0
C5 Isomerate	0		0	0
C6 Isomerate	0		0	0
C7-300 HC	0		41608	0
300-350 HC	0		13426	0
350-500 HC	0		0	61211
500-700 HC	0		0	130300
C7-300 HTU	0		0	0
300-350 HTU	0		0	0
350-500 HTU	0		0	0
500+ HTU	0		0	0
C5-C10 AN			61423	
H2O Produced	0		0	0
Total (Lb/hr)	*16580*	*1298*	*314637*	*191511*
Total (BPSD)	*2505*		*30288*	*16867*
Density (lb/ft3)				
Mol. Wt	*44.20*	*18.02*	*102.02*	*234.34*

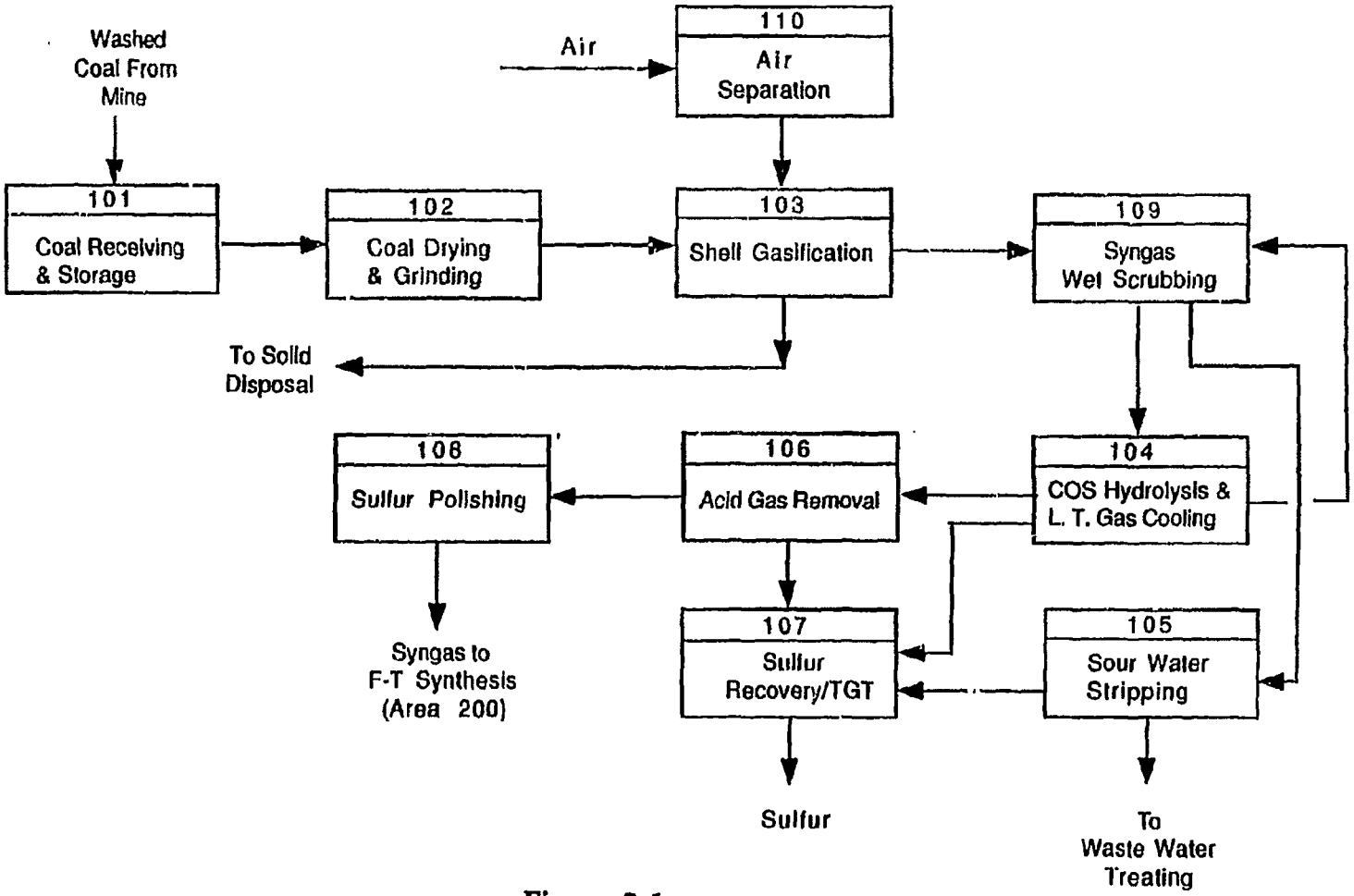


Figure 2-1

Block Flow Diagram - Area 100A (Syngas Production)

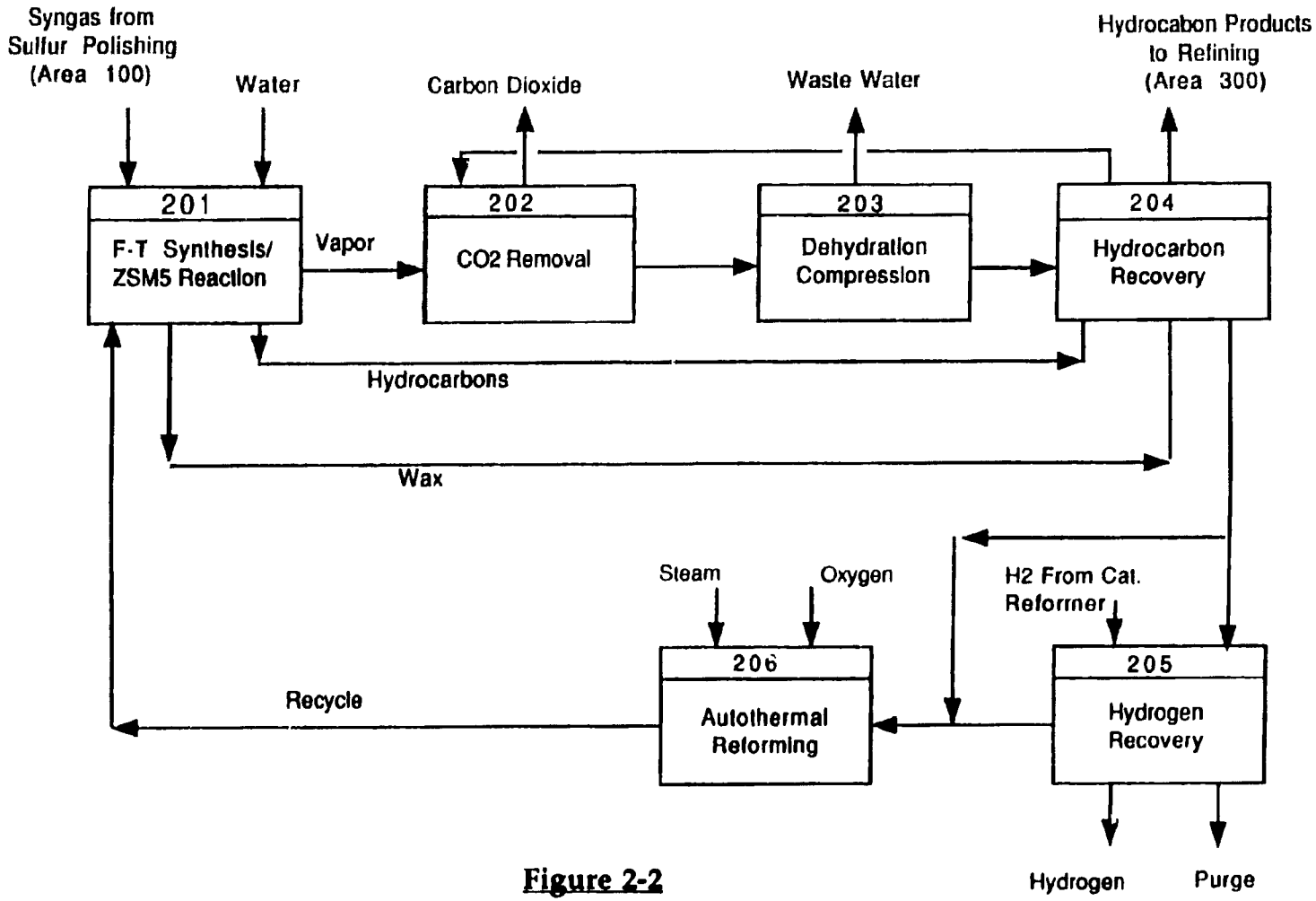


Figure 2-2

Block Flow Diagram - Area 200A (F-T Synthesis Loop)

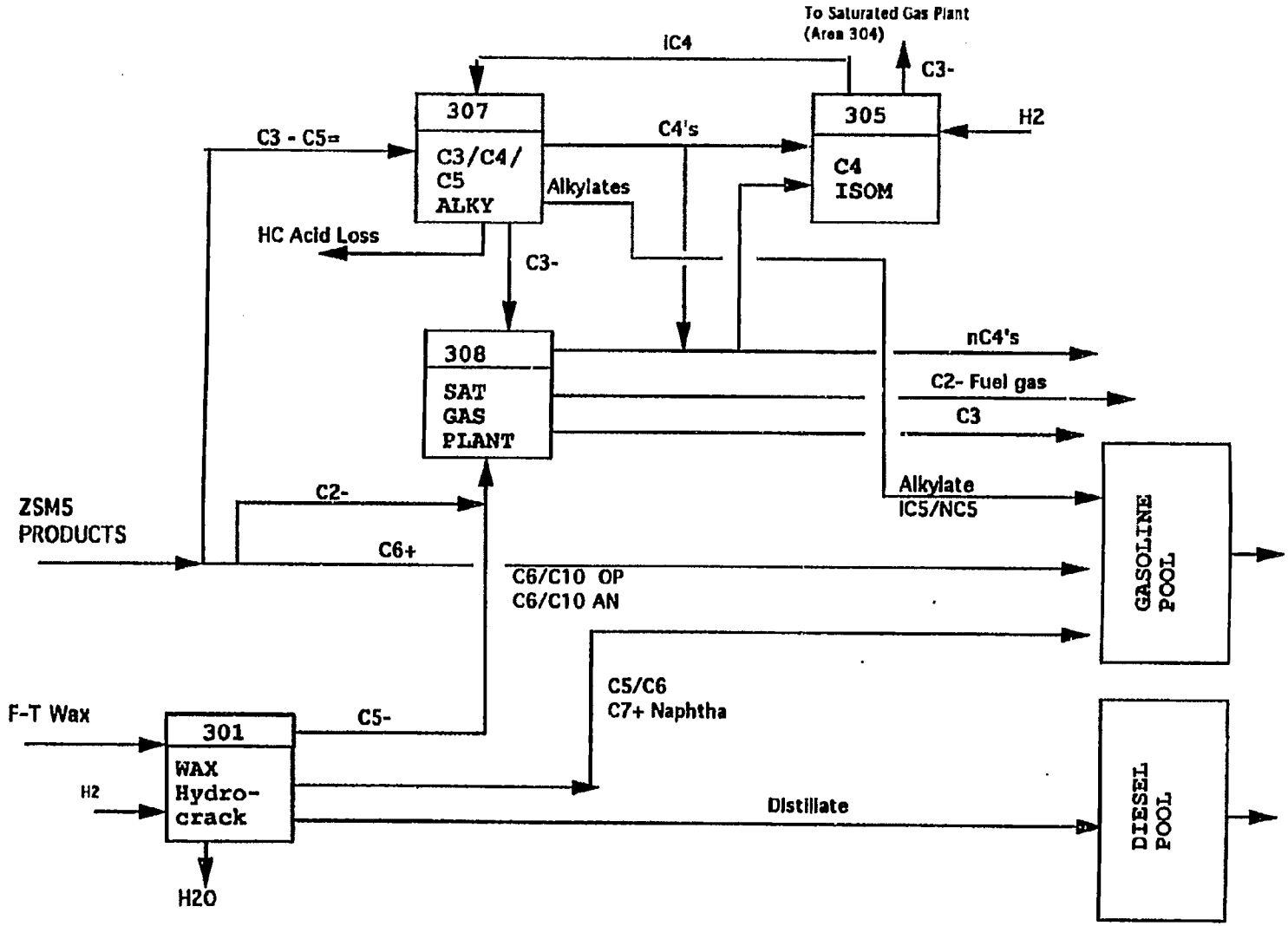
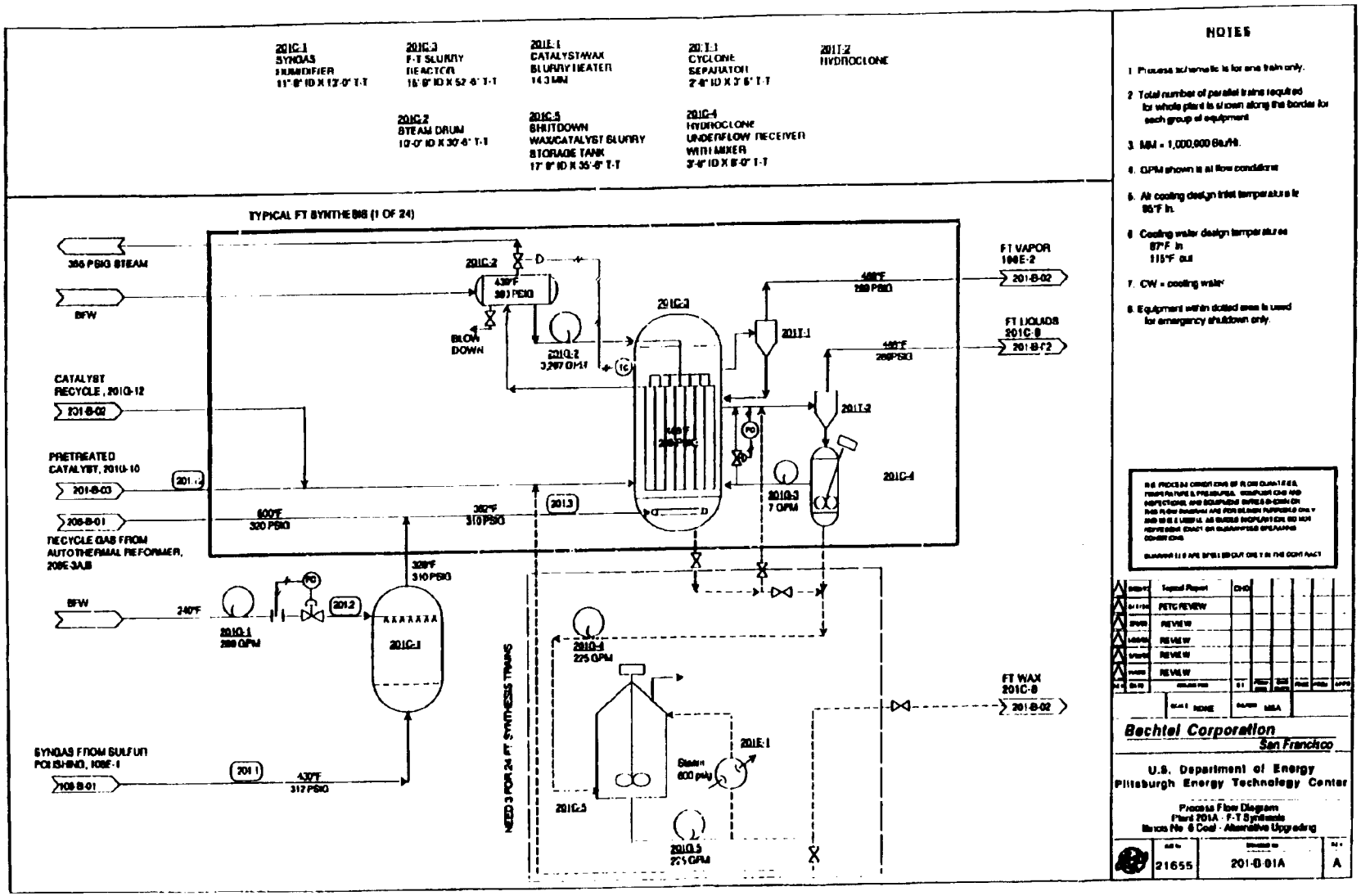


Figure 2-3

Block Flow Diagram - Area 300A F-T Product Upgrading



NOTES

1. Process schematic is for one train only.
2. Total number of parallel trains required for whole plant is shown along the border for each group of equipment.
3. MM = 1,000,000 Btu/Hr.
4. GPM shown is at flow conditions.
5. Air cooling design inlet temperature is 95°F in.
6. Cooling water design temperatures
   87°F in
   115°F out
7. CW = cooling water.
8. Equipment within dotted area is used for emergency shutdown only.

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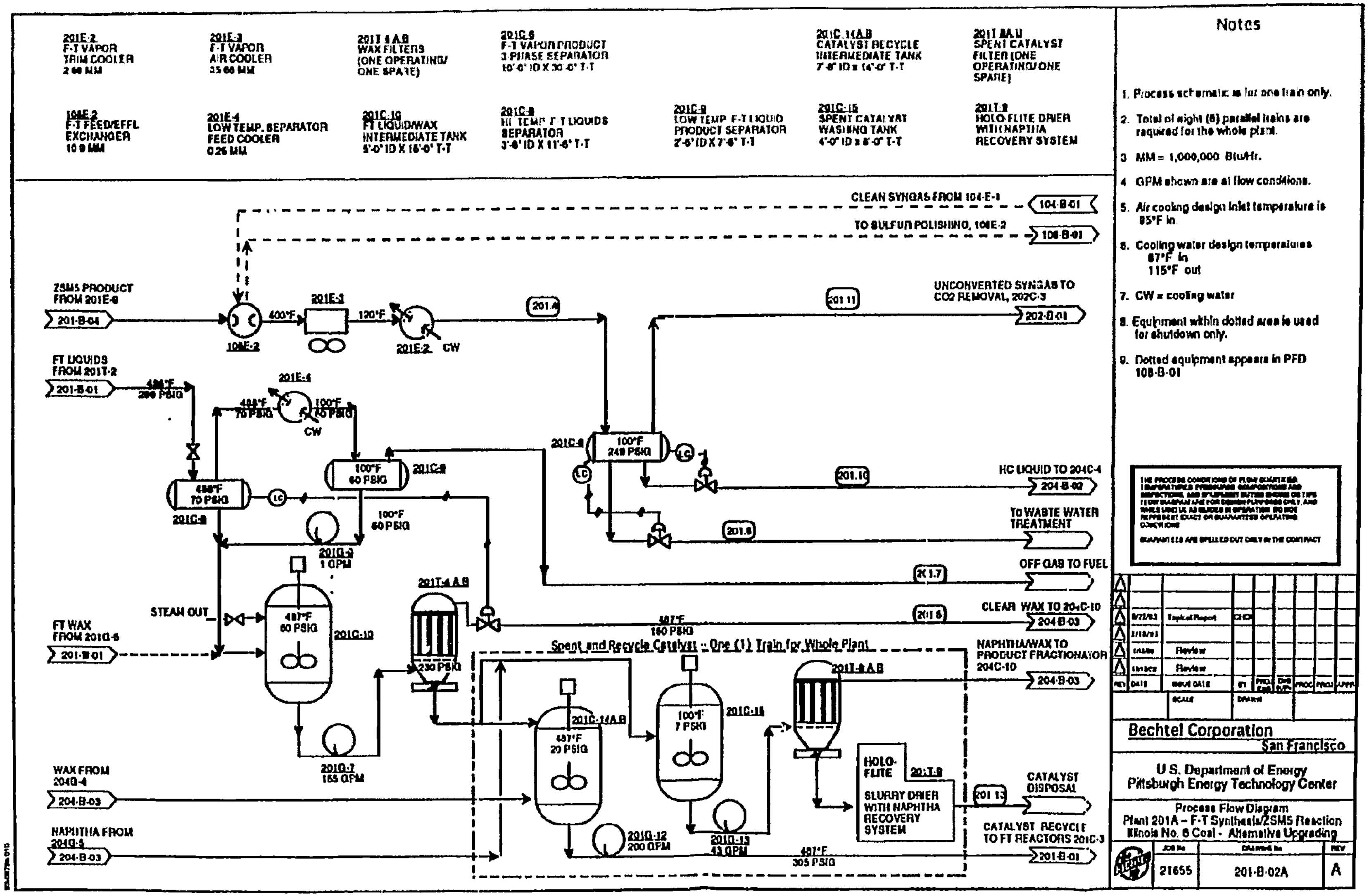
Bechtel Corporation
San Francisco

U.S. Department of Energy
Pittsburgh Energy Technology Center

Process Flow Diagram
Plant 201A - F-T Synthesis
Illinois No. 6 Coal - Alternative Upgrading

21655	201-B-01A	A


Notes
1. Process schematic is for one train only.
2. Total of eight (8) parallel trains are required for the whole plant.
3. MM = 1,000,000 Btu/Hr.
4. GPM shown are at flow conditions.
5. Air cooling design inlet temperature is 95°F in.
6. Cooling water design temperatures 87°F in 115°F out
7. CW = cooling water
8. Equipment within dotted area is used for shutdown only.
9. Dotted equipment appears in PFD 108-B-01
201E-2 F-T VAPOR TRIM COOLER
201E-3 F-T VAPOR AIR COOLER
201C-6 F-T VAPOR PRODUCT 3 PHASE SEPARATOR
201C-14A,B CATALYST RECYCLE INTERMEDIATE TANK
104E-2 F-T FEED/EFFL EXCHANGER
201E-4 LOW TEMP. SEPARATOR FEED COOLER
201C-10 FT LIQUID/WAX INTERMEDIATE TANK
201C-8 HI TEMP F-T LIQUIDS SEPARATOR
201C-9 LOW TEMP F-T LIQUID PRODUCT SEPARATOR
201C-15 SPENT CATALYST WASHING TANK
201T-9 HOLO-FLITE DRIER WITH NAPHTHA RECOVERY SYSTEM
CLEAN SYNGAS FROM 104-E-1
TO SULFUR POLISHING, 108E-2
ZSM5 PRODUCT FROM 201E-6
FT LIQUIDS FROM 201T-2
UNCONVERTED SYNGAS TO CO2 REMOVAL, 202C-3
HC LIQUID TO 204C-4
TO WASTE WATER TREATMENT
OFF GAS TO FUEL
CLEAN WAX TO 204C-10
FT WAX FROM 201C-6
STEAM OUT
Spent and Recycle Catalyst :- One (1) Train for Whole Plant
NAPHTHA/WAX TO PRODUCT FRACTIONATOR 204C-10
WAX FROM 204C-4
NAPHTHA FROM 204C-5
CATALYST DISPOSAL
CATALYST RECYCLE TO FT REACTORS 201C-3
HOLO-FLITE SLURRY DRIER WITH NAPHTHA RECOVERY SYSTEM
Bechtel Corporation
San Francisco
U.S. Department of Energy
Pittsburgh Energy Technology Center
Process Flow Diagram
Plant 201A – F-T Synthesis/ZSM5 Reaction
Illinois No. 6 Coal - Alternative Upgrading
21655
201-B-02A
A

201F-1
PRETREATER CIRCULATING GAS HEATER
4.8 MM

201C-11
CATALYST PRETREATER
12'-0" ID X 25'-0" T-T

201E-6
WAX HEATER
13.6 MM

201C-12
PRETREATED CATALYST FEED TANK
12'0" X 7'50" T-T

201T-6
MAKEUP CATALYST FEED HOPPER
220" X 44'-0" T-T

201K-1
PRETREATER CIRCULATING GAS COMPRESSOR
4501b³

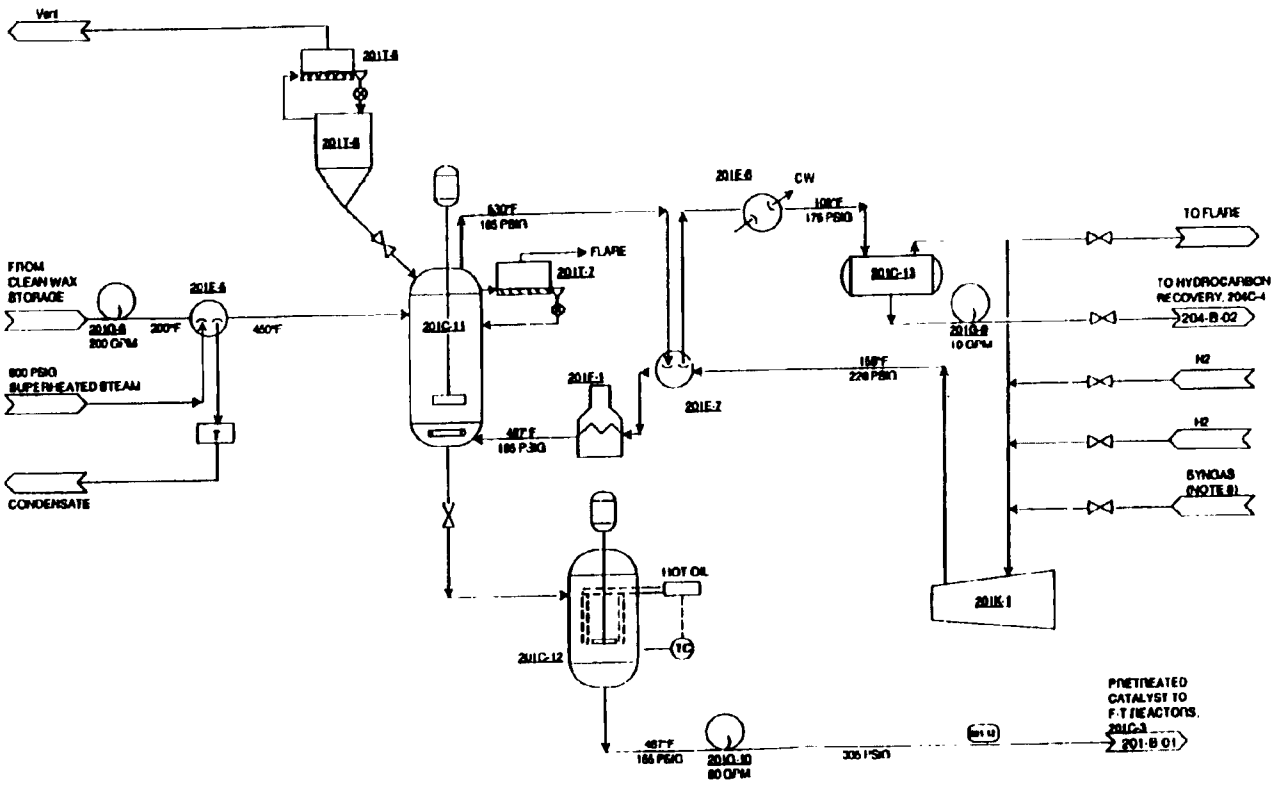
201T-5
MAKEUP CATALYST FEED HOPPER BAGHOUSE

201T-7
CATALYST PRETREATER BAGHOUSE

201E-8
CATALYST PRETREATER OVERHEAD COOLER
7.6 MM

201C-13
CATALYST PRETREATER OVERHEAD KO DRUM
4'0" X 8'-0" T-T

201E-7
PRETREATER FEED/EFFLUENT CROSS-EXCHANGER
5.7 MM



NOTES

1. One train for the whole plant
2. MM = 1,000,000 Btu/hr.
3. Air cooler design inlet temperature is 95°F in
4. Cooling water design temperatures
   87°F in
   115°F out
5. CW = cooling water
6. Catalyst pretreatment is a batch operation.
7. GPM shown is at flow conditions
8. 87,300 SCFH syngas usage during the reduction period

THE PROCESS CONDITIONS OF FLOW QUANTITIES, TEMPERATURES, PRESSURES, ... AND ENTHALPIES, AND DELINEATION ... THIS FLOW DIAGRAM ARE FOR DESIGN PURPOSES ONLY ... REPRESENT EXACT OR GUARANTEED OPERATING CONDITIONS

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Process Flow Diagram
Plant 201A · F-T Synthesis · Catalyst Pretreatment
Illinois No. 6 Coal · Alternative Upgrading

21655	201-B-03A	A

201K-2
ZSM-5 CATALYST REGENERATION AIR COMPRESSOR
2050 ACFM, 790 BHP

201E-2
ZSM-5 STARTUP HEATER (Note 10)
33.4 MM

201E-3
ZSM-5 REGENERATION GAS HEATER
1.9 MM

201C-16
ZSM-5 REACTOR
11'3" X 12'0" T-T

201E-10
ZSM-5 REGENERATION GAS EXCHANGER
33.5 MM

201E-8
ZSM-5 FEED/PRODUCT EXCHANGER
104.9 MM

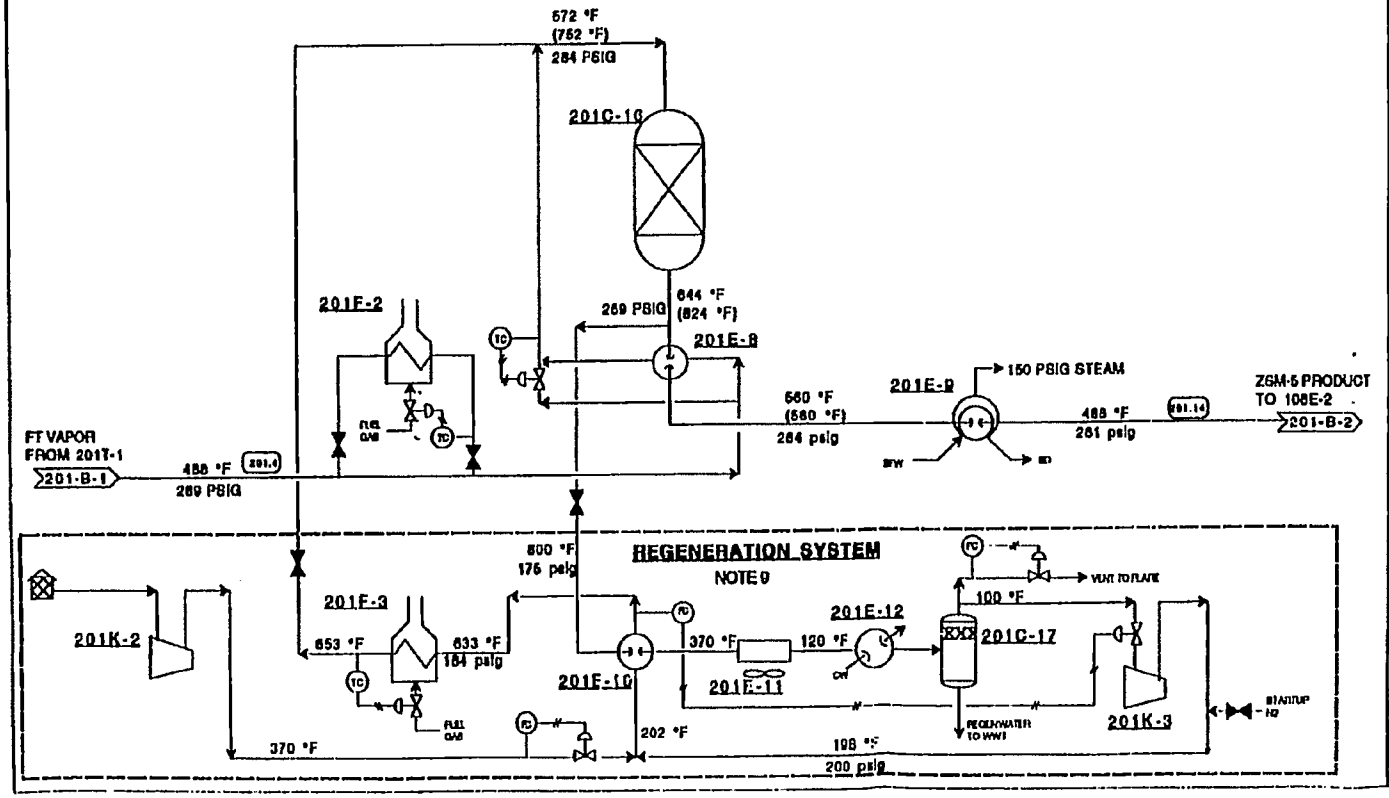
201E-11
ZSM-5 REGENERATION GAS AIR COOLER
19.3 MM

201E-9
ZSM-5 PRODUCT STEAM GENERATOR
28.6 MM

201E-12
ZSM-5 REGENERATION GAS WATER COOLER
1.5 MM

201C-17
ZSM-5 REGENERATION CONDENSATE SEPARATOR
9'0" x 13'0" T-T

201K-3
ZSM-5 CATALYST REGENERATION GAS COMPRESSOR
6570 ACFM, 2640 BHP



NOTES

1. Process schematic is for one train only.
2. A total of nine trains are required with eight operating and one in regeneration.
3. MM = 1,000,000 Btu/hr
4. GPM shown is at flow conditions
5. Air cooling design inlet temperature is 86°F in.
6. Cooling water design temperatures
   87°F in
   115°F out
7. CW = cooling water
8. Temperatures in parentheses refer to EOR conditions.
9. One regeneration system is required for the plant.
10. One startup heater is required for the plant.

THE PROCESS CONDITIONS OF FLOW QUANTITIES, TEMPERATURES, PRESSURES, COMPOSITIONS AND SIMULATIONS, AND EQUIPMENT OUTLINES SHOWN ON THIS FLOW DIAGRAM ARE FOR DESIGN PURPOSES ONLY, AND WHILE USEFUL AS GUIDES IN OPERATION, DO NOT REPRESENT EXACT OR GUARANTEED OPERATING CONDITIONS.

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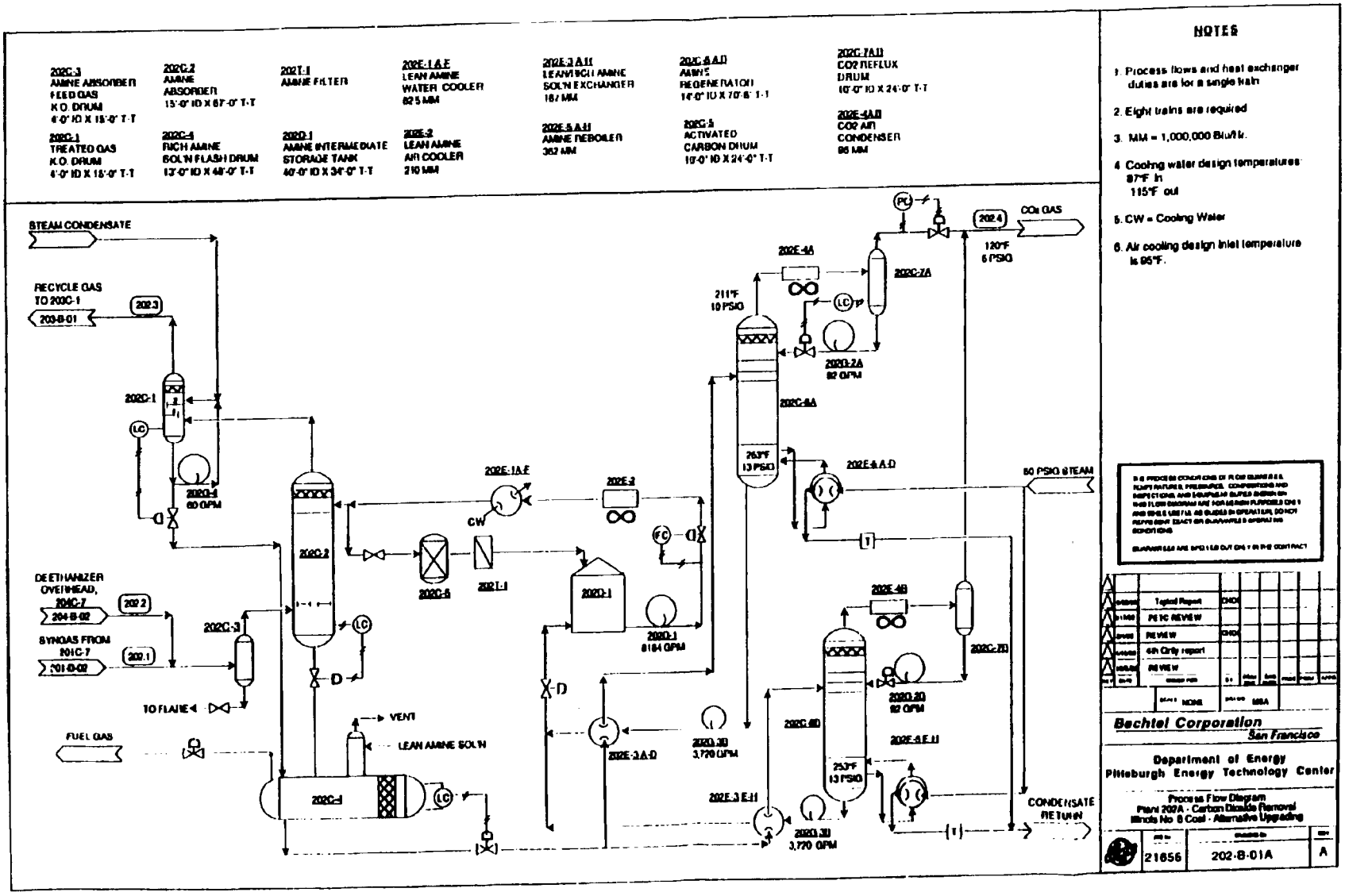
Process Flow Diagram
Plant 201A - F-T Synthesis/ZSM-5 Reaction
Illinois No. 6 Coal - Alternative Upgrading

21655	201-B 04A	A



NOTES

1. Process flows and heat exchanger duties are for a single train
2. Eight trains are required
3. MM = 1,000,000 Btu/hr.
4. Cooling water design temperatures
   87°F In
   115°F out
5. CW = Cooling Water
6. Air cooling design inlet temperature is 95°F.

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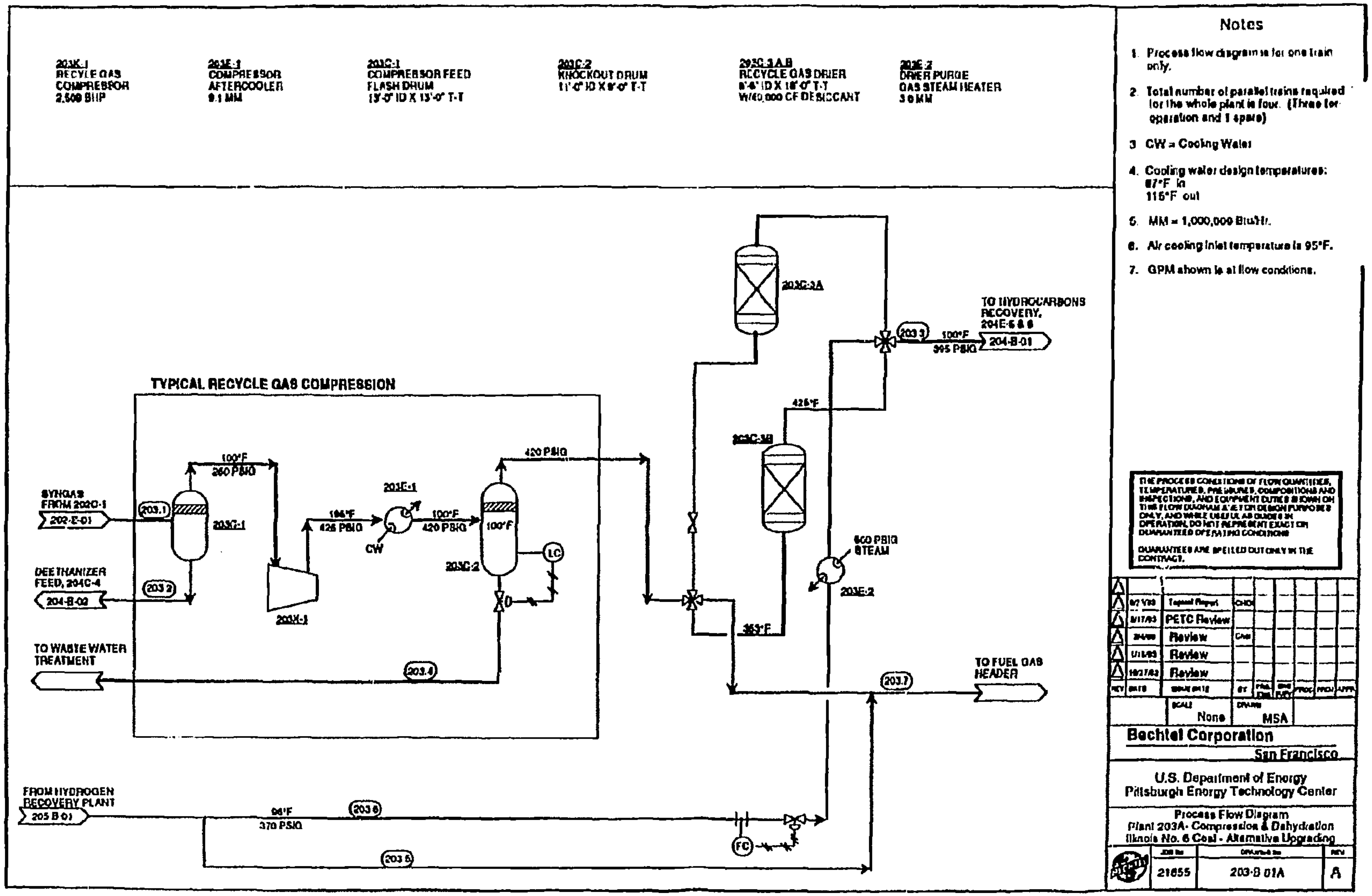
Process Flow Diagram
Plant 202A - Carbon Dioxide Removal
Illinois No 6 Coal - Alternative Upgrading

21656 | 202-B-01A | A



203K-1
RECYLE GAS
COMPRESSOR
2,500 BHP
203E-1
COMPRESSOR
AFTERCOOLER
9.1 MM
203C-1
COMPRESSOR FEED
FLASH DRUM
13'-0" ID X 13'-0" T-T
203C-2
KNOCKOUT DRUM
11'-0" ID X 8'-0" T-T
203C-3 A,B
RECYCLE GAS DRIER
8'-4" ID X 18'-0" T-T
W/40,000 CF DESICCANT
203E-2
DRIER PURGE
GAS STEAM HEATER
3.0 MM
TYPICAL RECYCLE GAS COMPRESSION
SYNGAS
FROM 202C-1
202-E-01
DEETHANIZER
FEED, 204C-4
204-B-02
TO WASTE WATER
TREATMENT
100°F
260 PSIG
196°F
426 PSIG
100°F
420 PSIG
420 PSIG
100°F
CW
LC
203C-3A
203C-3B
TO HYDROCARBONS
RECOVERY,
204E-5 & 6
100°F
395 PSIG
204-B-01
425°F
350°F
650 PSIG
STEAM
TO FUEL GAS
HEADER
FROM HYDROGEN
RECOVERY PLANT
205 B 01
96°F
370 PSIG
FC
203.1
203.2
203.3
203.4
203.5
203.6
203.7
Notes
1. Process flow diagram is for one train only.
2. Total number of parallel trains required for the whole plant is four. (Three for operation and 1 spare)
3 CW = Cooling Water
4. Cooling water design temperatures:
87°F in
115°F out
5. MM = 1,000,000 Btu/Hr.
6. Air cooling inlet temperature is 95°F.
7. GPM shown is at flow conditions.
PETC Review
Review
Review
Review
None
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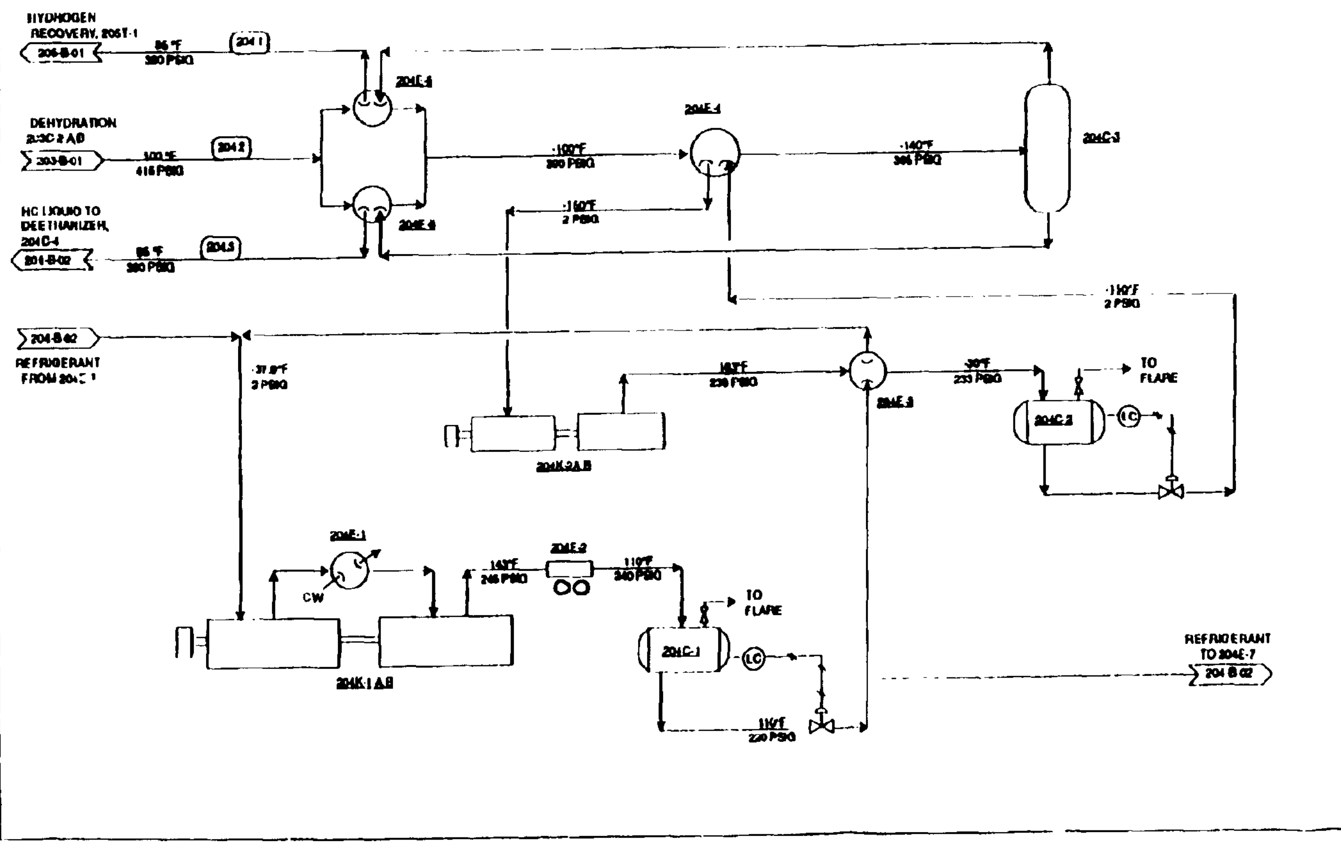
Process Flow Diagram
Plant 203A- Compression & Dehydration
Illinois No. 6 Coal - Alternative Upgrading
21655
203-B 01A
A

204K-1A,B PROPANE COMPRESSOR 1118 BHP EACH	204E-6 RECYCLE GAS/SEPARATOR LIQUID EXCHANGER 2.62 MM	204K-2A,B ETHYLENE COMPRESSOR 633 HP EACH	204C-3 RECYCLE GAS SEPARATOR 4'-0" ID X 8'-0" T-T	204E-2 PROPANE CONDENSER 11.6 MM	204C-2 ETHYLENE RECEIVER 5'-0" ID X 10'-0" T-T
204E-3 PROPANE/ETHYLENE EXCHANGER 6.1 MM	204E-5 RECYCLE GAS/SEPARATOR VAPOR EXCHANGER 7.0 MM		204C-1 PROPANE RECEIVER 7'-0" ID X 14'-0" T-T	204E-1 PROPANE COMPRESSOR INTERCOOLER 0.6 MM	204E-4 REFRIGERANT/RECYCLE GAS EXCHANGER 3.4 MM



NOTES

1. Process schematic is for one train only.
2. Total of four (4) trains are required for the whole plant.
3. CW = Cooling Water
4. Cooling water design temperatures 87°F in, 115°F out
5. GPM shown are at flow conditions.
6. MM = 1,000,000 Btu/Hr.
7. Air Cooling design inlet temperature is 95°F

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Process Flow Diagram
Plant 204A - Hydrocarbons Recovery
Illinois No. 6 Coal - Alternative Upgrading

21655 | 204-B-01A | A

204C-4
DEETHANIZER
6'-0" ID X 64'-0" T-T

204E-8
DEETHANIZER
REBOILER
9.9 MM

204C-6
SIDE DRAW
WATER DRUM
3'-0" ID X 7'-0" T-T

204E-9
DEPENTENIZER
CONDENSER
11.0 MM

204E-7
DEETHANIZER
CONDENSER
1.13 MM

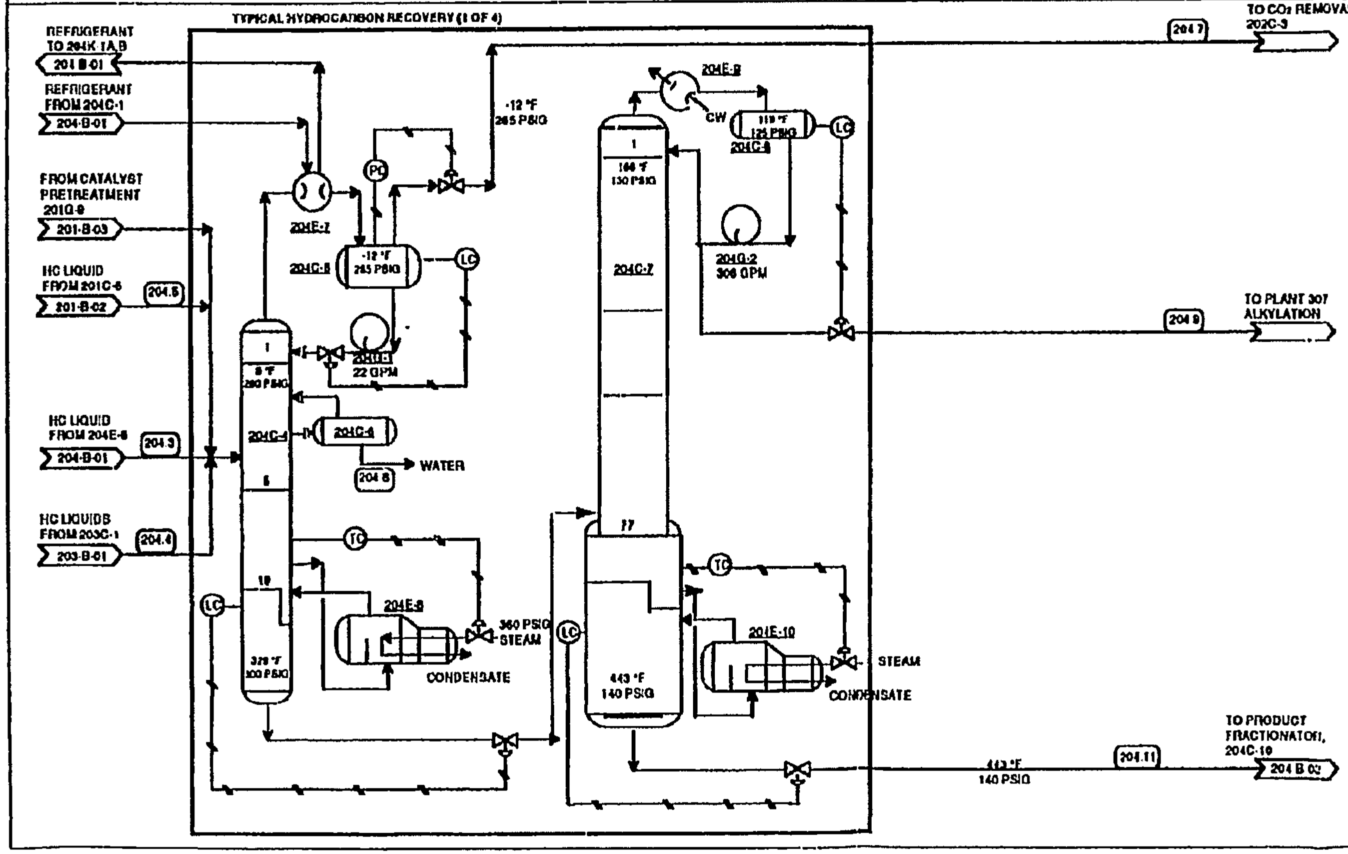
204C-7
DEPENTENIZER
5'-0" & 6'-0"ID X 103'-10" T-T

204C-5
DEETHANIZER
REFLUX DRUM
2'-6" ID X 7'-0" T-T

204C-8
DEPENTENIZER
REFLUX DRUM
4'-0" ID X 12'-0" T-T

204E-10
DEPENTENIZER
REBOILER
12.8 MM

TYPICAL HYDROCARBON RECOVERY (1 OF 4)



NOTES

1. Process schematic is for one train only.
2. MM = 1,000,000 Btu/Hr.
3. CW = Cooling Water
4. Air cooling design inlet temperature is 95 °F.
5. Cooling water design temperatures are 87 °F in and 116 °F out.
6. GPM shown is at flow conditions.

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	REVIEW	CHO	
	REVIEW		
	REVIEW		

SCALE NONE

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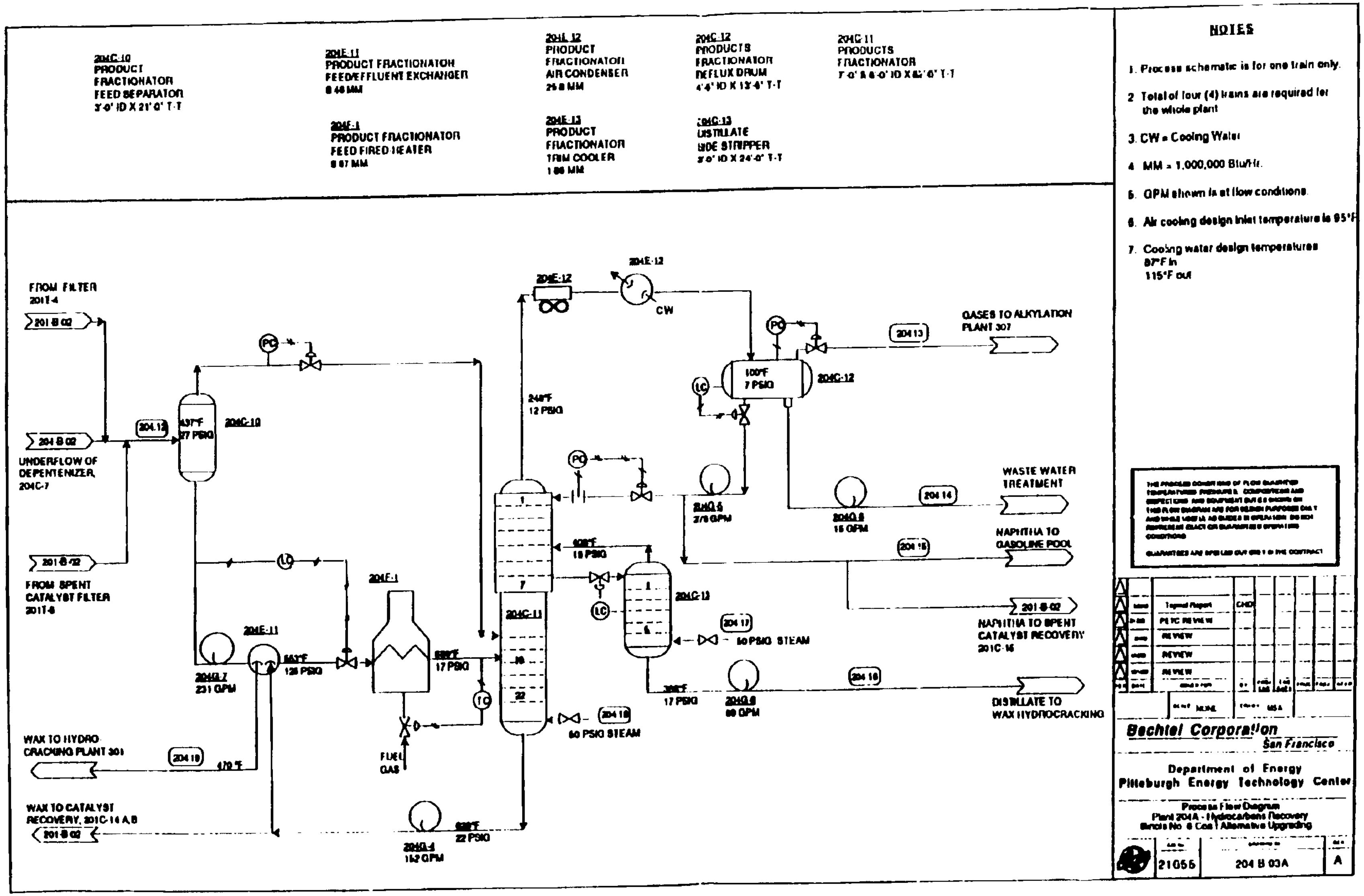
Process Flow Diagram
Plant 204A - Hydrocarbons Recovery
Illinois No. 6 Coal - Alternative Upgrading

21655	204-B 02A	A


204C-10
PRODUCT
FRACTIONATOR
FEED SEPARATOR
3'-0" ID X 21'-0" T-T
204E-11
PRODUCT FRACTIONATOR
FEED/EFFLUENT EXCHANGER
204F-1
PRODUCT FRACTIONATOR
FEED FIRED HEATER
204E-12
PRODUCT
FRACTIONATOR
AIR CONDENSER
204E-13
PRODUCT
FRACTIONATOR
TRIM COOLER
204C-12
PRODUCTS
FRACTIONATOR
REFLUX DRUM
204C-13
DISTILLATE
SIDE STRIPPER
204C-11
PRODUCTS
FRACTIONATOR
NOTES
1. Process schematic is for one train only.
2. Total of four (4) trains are required for the whole plant
3. CW = Cooling Water
4. MM = 1,000,000 Btu/Hr.
5. GPM shown is at flow conditions.
6. Air cooling design inlet temperature is 95°F
7. Cooling water design temperatures
87°F in
115°F out
FROM FILTER
201T-4
UNDERFLOW OF
DEPENTENIZER
204C-7
FROM SPENT
CATALYST FILTER
WAX TO HYDRO-
CRACKING PLANT 301
WAX TO CATALYST
RECOVERY, 201C-14 A,B
FUEL
GAS
CW
GASES TO ALKYLATION
PLANT 307
WASTE WATER
TREATMENT
NAPHTHA TO
GASOLINE POOL
NAPHTHA TO SPENT
CATALYST RECOVERY
201C-16
DISTILLATE TO
WAX HYDROCRACKING
50 PSIG STEAM
100°F
7 PSIG
17 PSIG
12 PSIG
22 PSIG
231 GPM
15 GPM
88 GPM
152 GPM
470 °F
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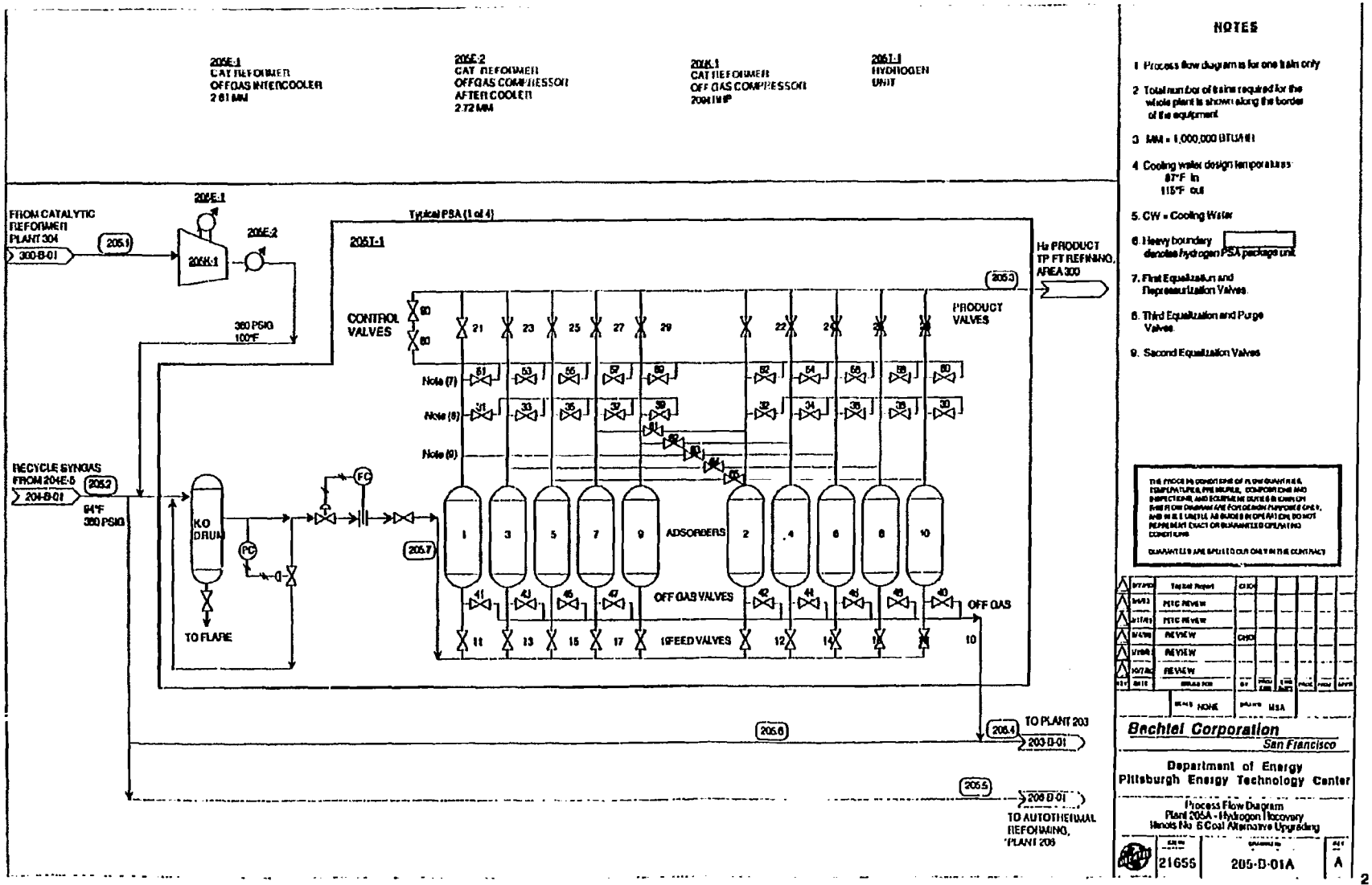
Process Flow Diagram
Plant 204A - Hydrocarbons Recovery
21055
204 B 03A
A



NOTES

1. Process flow diagram is for one train only
2. Total number of trains required for the whole plant is shown along the border of the equipment
3. MM = 1,000,000 BTU/HR
4. Cooling water design temperatures:
   87°F in
   115°F out
5. CW = Cooling Water
6. Heavy boundary denotes hydrogen PSA package unit
7. First Equalization and Repressurization Valves
8. Third Equalization and Purge Valves
9. Second Equalization Valves

THE PROCESS CONDITIONS OF FLOW QUANTITIES, TEMPERATURES, PRESSURES, COMPOSITIONS AND INSPECTIONS, AND EQUIPMENT DUTIES SHOWN ON THESE DIAGRAMS ARE FOR DESIGN PURPOSES ONLY, AND IN NO WAY LIMITS, AS GUIDES IN OPERATION, DO NOT REPRESENT EXACT OR GUARANTEED OPERATING CONDITIONS

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04/93	PETC REVIEW						
01/17/93	PETC REVIEW						
04/92	REVIEW	CHCH					
01/92	REVIEW						
10/27/92	REVIEW						
REV	DATE	ISSUED FOR	BY	CHKD	ENGR	PROJ	APPD

ISSUED FOR: NONE

APPD: MSA

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Process Flow Diagram
Plant 205A - Hydrogen Recovery
Illinois No. 6 Coal Alternative Upgrading

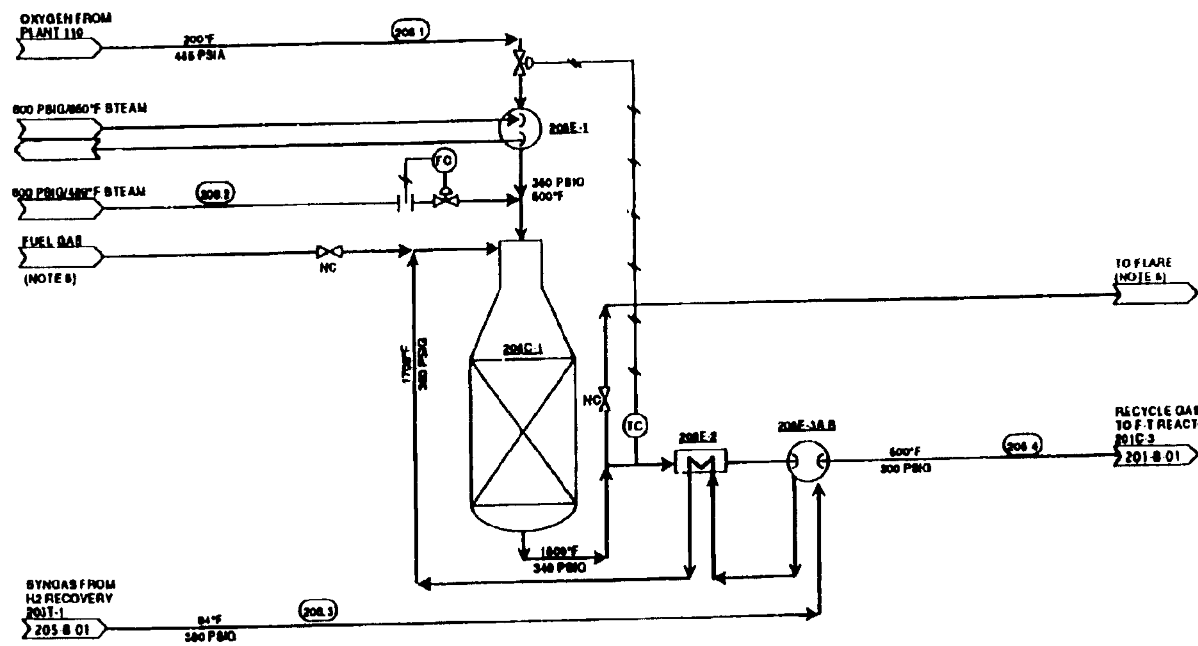
	21655	205-D-01A	A

206E-1
OXYGEN PREHEATER
0.8 MM

206C-1
AUTOTHERMAL REFORMER
7'-1" ID X 18'-0" T-T

206E-2
AUTOTHERMAL REFORMER
FEED SUPERHEATER
32.0 MM

206E-3A,B
AUTOTHERMAL REFORMER
FEED/EFFLUENT EXCHANGER
65.7 MM (TOTAL)



Notes

1. Process flows and heat exchanger duties are for one train only
2. Total of four (4) trains are required for the whole plant.
3. MM = 1,000,000 BTU/HR
4. NC = Normally closed
5. Fuel gas is used for start-up only.

REV	DATE	ISSUE DATE	BY					
		Topical Report	CHD					
		PETC Review						
		Review	CHD					
		4th Qtrly						
		Review						

SCALE: None
DRAWN: MSA

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Process Flow Diagram
Plant 206A - Autothermal Reformer
Illinois No. 6 Coal - Alternative Upgrading

JOB No.	DRAWING No.	REV
21655	206-D-01A	A

Section 3

Task 4 - Simulation Model Development

Previous quarterly progress reports described the development of preliminary ASPEN process simulation models for the individual plants in the indirect coal liquefaction complex and how they were integrated into three individual processing area models. One model for Area 100, the syngas production area; one model for Area 200, the Fischer-Tropsch synthesis reactor loop; and one model for Area 300, the conventional product refining area. During this quarter, some of the individual plant models were enhanced, additional models and routines were developed and these three area models were combined into a single ASPEN process simulation model of the entire indirect coal liquefaction complex for the baseline design case.

In addition, a separate model for the simplified product refining area, Area 300, of the alternate refining case was developed. In this alternate refining case, the primary product upgrading step is one in which the vapor leaving the Fischer-Tropsch reactors is passed over ZSM-5 catalyst. As a result, for the alternate refining case Area 300 contains fewer conventional petroleum refining units than are present in the baseline design case.

3.1 AREA 200 FISCHER-TROPSCH SYNTHESIS REACTOR LOOP MODELS

3.1.1 Plant 201, The Fischer-Tropsch Reactor Model

The basic Fischer-Tropsch spreadsheet reactor sizing model that is documented in the final report of the "Slurry Reactor Design Studies" (DOE project DE-AC22-89PC89867) was converted to Fortran code and integrated into the ASPEN process simulation model for Plant 201. The conversion of this spreadsheet model to Fortran was not simple because the calculation procedure involves several nested calculation loops. When these calculations are requested, the sizes of the Fischer-Tropsch slurry bed reactors will be calculated and reported.

The basic spreadsheet reactor sizing model was enhanced as it was converted and installed in the ASPEN process simulation model to provide a better prediction of the heat transfer as a function of the fluid velocity within the reactor. The original version of the model used a constant heat transfer coefficient that was independent of the slurry bed conditions.

This reactor sizing model now will allow the study of the effects of feed rate, feed composition, conversion, pressure, inlet gas velocity, catalyst concentration, catalyst makeup rate, and relative catalyst activity on the size of the slurry bed reactors. Eventually, this model will be extended to predict the reactor cost based on its size so that the effects on the reactor cost also can be studied.

3.1.2 Other Fischer-Tropsch Synthesis Loop Models

The previously developed ASPEN/SP Fortran user block models for Plants 202, 203, 204, 205, and 206 which predict the utilities consumptions and/or productions, operating personnel requirements, and ISBL plant costs as a function of capacity were added to the Area 200 model. The Fortran user block models are simple ones which have a single input stream and produce a single identical output stream. Based on the flow of this stream, they predict the utilities consumptions and/or productions, operating personnel requirements, and ISBL plant costs as a function of capacity.

Plant 202, the CO2 removal plant, was split into two sections for improved accuracy. Plant 202A is the amine absorption section for which the section cost is a function of the entering syngas flow rate, Plant 202B is the amine regeneration section for which the section cost is a function of the CO2 rejection rate. All the utilities consumptions for Plant 202 are attributed to Plant 202B, and consequently, are calculated as a function of the CO2 rejection rate.

The utilities consumptions and ISBL costs of Plant 203, the hydrogen compression plant; Plant 204, the hydrocarbon recovery plant; and Plant 206, the autothermal reforming plant, are calculated as a function of the entering syngas flow rate. The utilities consumptions and ISBL cost of Plant 205, the hydrogen recovery plant, are calculated as a function of the amount of hydrogen recovered.

Additional modifications also were made to some ASPEN flow splitter blocks to change some split specifications from an absolute basis to a relative basis so that various plant capacities can be studied.

3.2 PLANT 31, THE UTILITIES PLANT

A simplified Fortran user block model was developed for Plant 31, the utilities plant, to balance the steam productions and consumptions from all the process and other OSBL plants, to consume all the excess fuel gas, and to generate electric power. This model was developed only to balance the steam flows and to predict the electric power production so that an accurate prediction of the net electric power consumption for the entire complex can be made.

The Plant 31 utility plant model is a simplified one that is based on energy content. It does not simulate the individual pieces of equipment within the plant. It balances all the steam flows from the other plants by producing and/or consuming steam so that all the steam demands of the other plants are satisfied. If required, fuel gas is consumed to produce the steam consumed by the other plants. Any excess steam

and all remaining fuel gas are converted to electric power using an efficiency factor developed so that the model matches the design power production.

In addition, this model also reports a plant by plant and an overall utility summary for the entire coal liquefaction complex.

3.3 THE PLANT SIMULATION MODEL FOR THE BASELINE DESIGN CASE

The three individual and independent ASPEN process simulation models that were developed for Area 100, the syngas production area, Area 200, the Fischer-Tropsch synthesis reactor loop, and Area 300, the product refining (upgrading) area, were combined into a single model. Figure 3-1 schematically shows the major forward stream flows between these three areas. Not shown in Figure 3-1 are two recycle streams between areas. The major recycle stream is the hydrogen-rich light gas stream that goes from the naphtha catalytic reforming plant in Area 300 to the hydrogen recovery plant in Area 200. The other recycle stream is a small hydrogen stream that goes from the hydrogen recovery plant in Area 200 to the sulfur recovery plant in Area 100. Figures 3-2, 3-3 and 3-4 provide more detailed ASPEN block flow diagrams for Areas 100, 200 and 300, respectively.

The three processing areas are briefly described in the next three subsections. Following this is a subsection which describes how these three models are interconnected.

3.3.1 Area 100

Area 100, the syngas production area, contains ten process plants. Figure 3-2 is a block flow diagram showing the various ASPEN models and their interconnecting streams used to simulate Area 100. This processing area receives, grinds, dries and gasifies the coal to produce the syngas, and cleans the syngas before sending it to Area 200 for further processing. In addition this area contains a sour water stripping plant, sulfur recovery plant, and an air separation plant.

The ten processing plants in Area 100 are:

1. Plant 101, the Coal Receiving and Storage Plant
2. Plant 102, the Coal Grinding and Drying Plant
3. Plant 103, the Shell Gasification Plant
4. Plant 104, the Syngas Treating and Cooling Plant
5. Plant 105, the Sour Water Stripping Plant
6. Plant 106, the Acid Gas Removal Plant

7. Plant 107, the Sulfur Recovery and Tailgas Treating Plant
8. Plant 108, the Sulfur Polishing Plant
9. Plant 109, the Syngas Wet Scrubbing Plant
10. Plant 110, the Air Separation Plant

Area 100 is the only processing area of the coal liquefaction complex model in which solids may be present. The entering coal stream must be of ASPEN stream class MIXNC or MIXNCPSD and contain two substreams; one being a mixed substream of conventional components, and the other being a substream containing solid non-conventional components. All material streams entering and leaving the simulation blocks for Plants 101, 102, 103, and 109 also must be of the MIXNC or MIXNCPSD stream class. All entering and intermediate material streams associated with Plants 104 and 105 also must be of stream class MIXNC or MIXNCPSD. Those material streams leaving Plants 104 and 105 that require further processing pass through ASPEN stream class changer blocks to convert them to streams containing a single mixed substream of conventional components.

Each of the ten plant models in Area 100 was developed to simulate the specific plant only to provide sufficient detail to determine the major output streams, utilities consumptions, ISBL cost and number of operators as a function of the input streams. In many cases, wash water streams are neglected, and detailed combustion calculations are not performed to generate some flue gas streams. Utility balances are developed based on the detailed design, and their consumptions are calculated as linear functions of plant capacity.

The process simulation model for Area 100 contains no recycle streams as shown in Figure 3-2. However, the Area 100 model requires two ASPEN design specifications and six inline Fortran blocks. These are not shown in Figure 3-2.

The first design specifications is used to set the plant capacity. The user specifies the plant capacity by setting the moisture-free coal feed rate to Plant 103, the Shell coal gasification plant, in tons/day, and DES-SPEC FEEDRATE automatically adjusts the entering mine coal feed rate to the plant in stream MINECOAL to obtain this desired gasifier feed rate.

The other design specification, DES-SPEC O2PLANT, matches the oxygen production in Plant 110 to the total oxygen consumption by adjusting the air feed rate to Plant 110.

The six inline Fortran blocks are used essentially as feed-forward controllers. Fortran block MOIST maintains the moisture level of the inlet ROM coal in stream MINECOAL as its flow rate is varied by DES-SPEC FEEDRATE. The other five Fortran blocks are used to set the flow rates of various inlet streams to several plants

as a function of plant capacity. Fortran block SETUP103 sets the inlet oxygen and carbon dioxide stream flow rates to Plant 103. Fortran blocks SETUP104, SETUP106 and SETUP109 set the inlet water flow rate to Plants 104, 106 and 109, respectively, as a function of plant capacity. Fortran block SETUP107 sets the inlet hydrogen (reducing gas) rate to Plant 107 as a function of capacity.

3.3.2 Area 200

Area 200, the Fischer-Tropsch synthesis area, contains seven process plants. For the baseline design case, only six are functioning plants. The seventh plant, Plant 107, is the ZSM-5 reaction area, and it only functions in the model of the alternate refining case. This processing area takes the clean syngas from Plant 108 and processes it to produce hydrogen, fuel gas, light gaseous products, liquids and wax. These products are further processed in Area 300, the product refining area, to gasoline and diesel fuel.

Figure 3-3 is a block flow diagram showing the various ASPEN models and their interconnecting streams used to simulate Area 200. Forty-six ASPEN blocks are used to simulate the seven process plants. This model is a slightly simplified version of the one that was used to develop the baseline design.

The process plants in the process simulation model for Area 200 are:

1. Plant 201, the Fischer-Tropsch Synthesis Plant
2. Plant 202A, the Amine Absorption Section of the Carbon Dioxide Removal Plant
3. Plant 202B, the Amine Regeneration Section of the Carbon Dioxide Removal Plant
4. Plant 203, the Recycle Gas Compression and Dehydration Plant
5. Plant 204, the Hydrocarbon Recovery Plant
6. Plant 205, the Hydrogen Recovery Plant
7. Plant 206, the Autothermal Reforming Plant
8. Plant 207, the ZSM-5 Oligomerization Plant

Plant 202, the CO2 removal plant, was split into two sections for improved accuracy. Plant 202A is the amine absorption section, and Plant 202B is the amine regeneration section. By splitting this plant into two sections, the model will be more responsive to changes in the gas composition and flow rate within the Fischer-Tropsch synthesis loop.

All streams in the area 200 section of the model are of the ASPEN stream class MIXED and contain only one substream of conventional components. No solid non-conventional components may be present in this processing area.
Again, each of the seven plant models in Area 200 was developed to simulate the specific plant only to provide sufficient detail to determine the major output streams, utilities consumptions, ISBL cost and number of operators as a function of the input streams. Utility balances are developed based on the detailed design, and their consumptions calculated as linear functions of plant capacity.

The process simulation model for Area 200, the Fischer-Tropsch recycle loop, contains two recycle streams. These recycle streams are streams 204S5 and 206S4. Only one ASPEN convergence block is required to converge both of these recycle streams. Convergence block FTL1 converges both of these recycle streams using stream 202S3 as the single tear stream using the Wegstein convergence procedure.

The process simulation model for Area 200 requires one ASPEN design specification and three inline Fortran blocks. These are not shown in Figure 3-3.

The hydrogen production from Plant 205 is adjusted by ASPEN design specification H2MAKE so that it exactly satisfies the hydrogen demand in Areas 100 and 300. Convergence block H2MAKE, which contains the processing blocks for both Areas 200 and 300, balances the hydrogen production against the hydrogen demand by adjusting the amount of gas withdrawn from the F-T recycle loop and sent to Plant 205, the hydrogen recovery plant.

Fortran block SETUP201 acts as a feed-forward controller to set the inlet steam flow rate to Plant 201 as a function of the inlet syngas feed rate and composition. Fortran block SETUP21A sets the temperature of ASPEN flash block P201S1 to be the same as that of the Fischer-Tropsch synthesis reactor effluent stream so that block P201S1 simulates the inter-reactor vapor-liquid separation. Fortran block SETUP206 sets the inlet oxygen and steam flow rates to the autothermal reforming plant, Plant 206, as a function of the entering gas flow rate.

3.3.2 Area 300

Area 300, the Fischer-Tropsch product upgrading and refining area, contains eight process plants. These are standard petroleum refining units which use conventional technologies to upgrade and refine the hydrocarbons produced in Area 200 to high quality transportation fuels.

Figure 3-4 is an ASPEN block flow diagram showing the various ASPEN models and their interconnecting streams used to simulate Area 300, the product upgrading

and refining area for the baseline design. Nineteen ASPEN blocks are used to simulate the eight process plants. This model is a simplified one which employs Fortran user block models containing empirical, elementally balanced yield models to simulate all of the conversion processes and predict the utilities consumptions and ISBL costs of the plants. Not shown in this figure are six inline Fortran blocks which set the flow rates of the purchased butanes and makeup hydrogen streams to the various plants.

The eight process plants in Area 300 are:

1. Plant 301, the Wax Hydrocracking Plant
2. Plant 302, the Distillate Hydrotreating Plant
3. Plant 303, the Naphtha Hydrotreating Plant
4. Plant 304, the Naphtha Catalytic Reforming Plant
5. Plant 305, the C4 Isomerization Plant
6. Plant 306, the C5/C6 Isomerization Plant
7. Plant 307, the C3/C4/C5 Alkylation Plant
8. Plant 308, the Saturated Gas Plant

In the ZSM-5 alternate refining case, only four of the above eight plants are required. Plants 302, 303, 304, and 306 not needed since the ZSM-5 oligomerization reactor in Plant 207 is the primary product upgrading step. The development of the flowsheet for Area 300 of the alternate refining case will be discussed later.

All streams in the Area 300 section of the model are of the ASPEN stream class MIXED and contain only one substream of conventional components. No solid non-conventional components may be present in this processing area.
Again, each of the eight plant models was developed to simulate the specific plant only to provide sufficient detail to determine the major output streams and their qualities, utilities consumptions, ISBL cost and number of operators as a function of the input streams. Utility balances are developed based on the detailed design, and utility consumptions are calculated as linear functions of plant capacity.

For the baseline design case, the process simulation model for Area 300 contains a single recycle stream. It also requires six inline Fortran blocks. These are not shown in Figure 3-4.

The single recycle stream within Area 300 is stream 308S1, which is the butanes stream from Plant 308 that is returned to Plant 305, the C4 isomerization plant. This recycle loop only encompasses three plants, Plants 305, 307 and 308. ASPEN convergence block C4FLO converges this recycle loop using stream 308S1. As this loop is converged, inline Fortran block SETUP307 simultaneously adjusts the flow

rate of the purchased butanes going to block P305M to maintain the specified isobutane/olefin ratio in the feed to the alkylation plant, Plant 307.

In the ZSM-5 alternate refining case, excess butanes are produced, and no additional butanes must be purchased. Therefore, a different convergence procedure is required. This convergence procedure will be subsequently described when the ZSM-5 alternate refining model is discussed.

The five other inline Fortran blocks in Area 300, SETUP301, SETUP302, SETUP303, SETUP305, and SETUP306, set the flow rates of the inlet hydrogen streams to Plants 301, 302, 303, 305, and 306, respectively. All the inline Fortran blocks are not shown in Figure 3-4

There is one recycle stream between Areas 200 and 300. The hydrogen-rich C2 and lighter gas stream from the naphtha reforming plant (stream 304S2) is sent to Plant 205 for hydrogen recovery. ASPEN convergence block REFMRH2 converges this recycle loop using stream 304S2 as the tear stream by the Wegstein method.

As discussed in subsection 3.3.2, the hydrogen production from Plant 205 is adjusted by ASPEN design specification H2MAKE so that it exactly satisfies the hydrogen demand in Areas 100 and 300. Convergence block H2MAKE, which contains the processing blocks for both Areas 200 and 300 and the REFMRH2 convergence block, balances the hydrogen production against the hydrogen demand by adjusting the amount of gas withdrawn from the Fischer-Tropsch recycle loop that goes to Plant 205, the hydrogen recovery plant.

3.3.4 Overall Description

The overall process simulation model for the baseline design basically is the combination of the previously discussed flowsheets, shown in Figures 3-2, 3-3 and 3-3 for process Areas 100, 200 and 300, respectively.

In reality, three streams flow between Area 100 and Area 200; whereas in the model, there is only one. Stream 108S2 is the clean syngas from the sulfur polishing plant, Plant 108, that goes to the Fischer-Tropsch synthesis plant, Plant 201. The second is a small oxygen stream from the air separation plant, Plant 110, which goes to Plant 206, the autothermal reforming plant. The third stream is a small recycle stream consisting of a portion of the hydrogen pproduct from Plant 205 that is used as reducing gas in the sulfur plant, Plant 107.

Since Plant 205, the hydrogen recovery plant, produces an essentially pure hydrogen stream, no direct coupling of the hydrogen recycle stream to Plant 107 is needed

since it's composition is known. After all the plants in Area 100 except for Plant 108 have been solved, the sulfur recovery plant is solved because the flow rate of the hydrogen reducing gas is assumed to be proportional to the amount of sulfur entering the plant. Thus, when the calculations reach Area 200, the amount of hydrogen consumed in Plant 108 only has to be included in the calculations for the amount of hydrogen that is available for other uses.

A similar procedure also is employed to size Plant 110, the air separation plant, since again the composition of the oxygen stream is known, but its flow rate is not. Thus, after the oxygen demand from Plants 103 and 206 has been calculated, it is a simple matter to size Plant 110 to satisfy this oxygen demand. ASPEN design specification O2PLANT is used to balance the oxygen production from the air separation plant against the oxygen demand.

Several streams flow between Area 200 and Area 300. Four hydrocarbon product streams and five hydrogen streams flow forward from Area 200 into Area 300. However, there is only one recycle stream back to Area 200, and that is Stream 304S2, the hydrogen-rich product gas from the naphtha reforming plant, Plant 304, that goes to the hydrogen recovery plant.

ASPEN convergence block REFMH2 converges this recycle loop by the Wegstein method using stream 304S2 as the tear stream.

For the alternate refining case using ZSM-5 catalyst, Area 300 does not contain a naphtha reforming plant, and there is no hydrogen-rich stream which is recycled back to Area 200. Consequently, convergence block REFMH2 is not present.

The hydrogen produced by Plant 205 is used in Plants 107, 301, 302, 303, 305, and 306. The amount of hydrogen produced is controlled by feed rate to the plant, which is set by the split fraction in the ASPEN stream splitter block P205S1. Again, since Plant 205 produces essentially pure hydrogen, it is not necessary to connect the hydrogen streams. After the total hydrogen consumption in Plants 107, 301, 302, 303, 305, and 306 is known, it is only necessary to make Plant 205 produce the correct amount of hydrogen by adjusting the split fraction in block P205S1. An ASPEN design specification around both Areas 200 and 300 is used to balance the hydrogen production against the hydrogen consumption. DES-SPEC H2MAKE varies the split fraction in block P201S1 so that the hydrogen produced by Plant 205 in stream 205S3 matches the hydrogen consumption by the other plants. Convergence block H2MAKE is used to converge this design specification.

After the entire simulation model has been converged and all stream flow rates and compositions are known, Fortran block SUMMARY is executed. This inline Fortran block controls the final summarizing calculations and calls several subroutines to

do these calculations. This block calculates the properties of the blended gasoline and diesel products, utilities balance, total plant cost, and the catalyst and chemicals cost. It also writes the management summary report portion of the plant summary report file and the ICL.PRN output file for transfer of the model results to the Lotus spreadsheet Economics model.

In addition, there are several ASPEN mixing blocks in the model that are not shown in Figures 3-2, 3-3 and 3-4. These mixing blocks calculate the total sour water production in Areas 200 and 300 and the total fuel gas production by the entire plant.

3.3.5 Simulation Model Results for the Baseline Design Case

The output from the model that is of interest to the user is contained in several output files, the standard ASPEN report file, two ASPEN history files, the plant summary report file (the ALL.REP file), and the ASCII transfer file (the ICL.PRN file).

The standard ASPEN report file basically reports how the simulation progressed and provides the block and stream reports. The stream report contains the flow rates and compositions of all the streams as specified in the STREAM-REPORT paragraphs of the ASPEN input file. The .HIT file is a history of the progress of the ASPEN input translation step. This file contains two listings of the input file, one raw and one sorted, details on the component properties and thermodynamic models which are being used, and the calculation sequence which will be employed. The .HSP file is the history file produced during execution of the model. Supplemental output generated by the individual plant Fortran user block models as requested by the user are printed to this file. Near the end of this file, the calculated properties of the gasoline and diesel products are printed by inline Fortran block SUMMARY.

In addition to the above standard ASPEN output files, the model produces a Plant Summary Report file. This file was developed to summarize the individual plant operations in an easy to read manner in a standard format on a single page whenever possible.

The second page of the Plant Summary Report file contains the management summary report which summarizes the entire model results on a single page as shown in Figure 3-5. A summary of the major plant input and output streams is given at the top of the page. The middle section of the page provides a summary of the individual plants. This includes the number of operating and spare plants, the number of dedicated operators, the ISBL cost, and the total installed plant cost. The total installed cost includes an apportioned amount for the OSBL cost, home office

cost, fees, and contingency. The total number of operators, foremen and maintenance workers are given at the bottom of the page.

The remainder of the report contains short summaries (single page whenever possible) of the individual plant operations and an overall utilities summary table. Generally, these plant reports summarize the inlet and outlet stream flows, utilities consumptions or productions, and the ISBL field cost. A utilities summary table is given an the end of the Plant Summary Report which shows the steam, power, fuel, cooling water, process water and nitrogen consumptions or productions of the individual process and OSBL plants.

Table 3.1 compares the model results with those of the process design for the baseline design case. The agreement is excellent. The small differences between the model and the process design are the result of minor revisions and improvements which were made to the Fischer-Tropsch synthesis reactor model and some of the refining plant models in Area 300 after the process design was stabilized.

3.4 THE ALTERNATE REFINING CASE PROCESS MODEL FOR AREA 300

3.4.1 Overview

A separate process simulation model was developed for Area 300 of the alternate refining case where the Fischer-Tropsch reactor vapors are upgraded by passing them through a rector containing ZSM-5 oligomerization catalyst. In this configuration, all of the overhead vapor from the slurry phase Fischer-Tropsch reactor is passed directly to a second stage, fixed bed reactor containing ZSM-5 catalyst where olefins, oxygenates and heavy paraffins are converted to a mixture of isoparaffins, isoolefins, naphthenes and aromatics. All of the oxygen atoms in the oxygenates are converted to water. The C5+ portion of this product is a quality gasoline and the light ends are converted to gasoline by alkylation. The wax fraction is hydrocracked to produce naphtha and distillate.

As a result of the improved gasoline quality, the configuration of the Area 300 refining section for the alternate refining case is different. It contains only the following four plants.

1. Plant 301, the Wax Hydrocracking Plant
2. Plant 305, the C4 Isomerization Plant
3. Plant 307, the C3/C4/C5 Alkylation Plant
4. Plant 308, the Saturated Gas Plant.

The distillate hydrotreating, naphtha hydrotreating, naphtha reforming, and C5/C6 isomerization plants have been eliminated. This configuration produces more butanes than are consumed by the alkylation unit. These extra butanes are now sold, in contrast to the baseline design case which was short of butanes and had to purchase them.

In order to avoid confusion with the baseline design case, the four product streams produced by the Fischer-Tropsch synthesis loop and sent to Area 300 for further processing have been renumbered. These four streams are:

1. Stream 204S31, a C3-C5 olefin/paraffin stream going to the alkylation plant
2. Stream 204S32, a light gases stream going to the saturated gas plant
3. Stream 204S33, a naphtha stream which goes to gasoline blending
4. Stream 204S34, a distillate and wax stream which goes to the wax hydrocracker

In the baseline design case, all the C5 and lighter material is sent to the alkylation plant for further separation and processing, the naphtha stream is sent to the naphtha hydrotreater, and the distillate stream is sent to a distillate hydrotreater. The product refining area, Area 300, is completely different for the alternate refining case. It only contains four processing plants compared to the eight in the baseline design case. Figure 3-6 shows the ASPEN block flow diagram for the Area 300 product refining area for the alternate refining case. In this case, the C5 and lighter stream is split in Plant 204 to produce an alkylate feed stream and a light gas stream which goes to Plant 308, the saturated gas plant. The naphtha stream goes directly to gasoline blending. However, in this case, the material that was previously in the C5/C6 and naphtha product streams goes directly to gasoline blending rather than for further processing in the C5/C6 isomerization and naphtha reforming plants, respectively. The wax stream still goes to the wax hydrocracker.

The configuration of the model for the loop containing Plants 304, 307 and 308 is different from the baseline design for this case because extra butanes are available. Plant 308 now produces a stream named C4SELL from block P308M4 which represents the extra butanes that are sold. In the baseline design case, Plant 305 has an input stream named C4BUY which represents the butanes purchases. The Plant 307 alkylation plant model now contains another block, block P307S, which splits the excess normal butane between that going to the C4 isomerization plant and butane sales.

In the baseline design case, all butanes which could be recovered by Plant 308, the saturated gas plant, are sent to the C4 isomerization plant to minimize butane

purchases. In this case, only the isobutane is returned to the alkylation plant via the C4 isomerization plant, and the normal butanes are sold.

In the baseline design case, ASPEN convergence block C4FLOW works in conjunction with inline Fortran block SETUP307 to calculate the correct makeup butane flow rate in stream C4BUY to satisfy the butane demand of the alkylation plant. In this alternate refining case, convergence block C4FLOW works in conjunction with an ASPEN design specification to satisfy the butane demand of the alkylation plant and calculate the butane sales rate in stream C4SELL. This design specification sets the split fraction in block P307S, which controls the amount butane going to the C4 isomerization plant, to maintain the correct isobutane/olefin consumption ratio in the alkylation unit. An ASPEN convergence block is required to converge this design specification. Both the design specification and convergence block are not shown in Figure 3-6.

TABLE 3-1

Comparison of the ASPEN/SP Process Simulation
Model with the Process Design for the
Baseline Design Case

	Model	Design	Delta (M-D)	Percent Delta
ROM COAL FEED RATE, MTSD (MF)	18.575	18.575	0	0
COAL CLEANING REFUSE RATE, MTSD (MF)	0	0	0	0
SLAG PRODUCTION RATE, MTSD (MF)	2.244	2.244	0	0
NATURAL GAS RATE, MMMBTU/SD	0	0	0	0
ELECTRICITY PURCHASE, MEGA-WH/SD	1198.37	1198.54	-0.17	-0.14
RAW WATER MAKE-UP, MMGSD	14.460	14.460	0	0
GASOLINE PRODUCTION, MBSD	23.952	23.915	0.037	0.16
DIESEL PRODUCTION, MBSD	24.681	24.655	0.026	0.10
FUTURE PRODUCT A PRODUCTION, MBSD	0	0	0	0
FUTURE PRODUCT B PRODUCTION, MBSD	0	0	0	0
LIQUID PROPANE PRODUCTION, MBSD	1.923	1.921	0.002	0.10
MIXED BUTANES PRODUCTION, MBSD	-3.121	-3.119	-0.002	0.06
FUTURE BYPRODUCT C PRODUCTION,MTSD	0	0	0	0
FUTURE BYPRODUCT D PRODUCTION,MTSD	0	0	0	0
SULFUR PRODUCTION, MTSD	0.560	0.560	0	0
OPERATORS AND MAINTENANCE WORKERS	1088	1088	0	0
TOTAL INSTALLED CAPITAL, $MM(E-YR)	2906.55	2906.39	0.16	0.006
CATALYST AND CHEMICALS, $MM(B-YR)	31.07	31.07	0	0

Figure 3-1

BASELINE DESIGN
OVERALL PROCESS CONFIGURATION

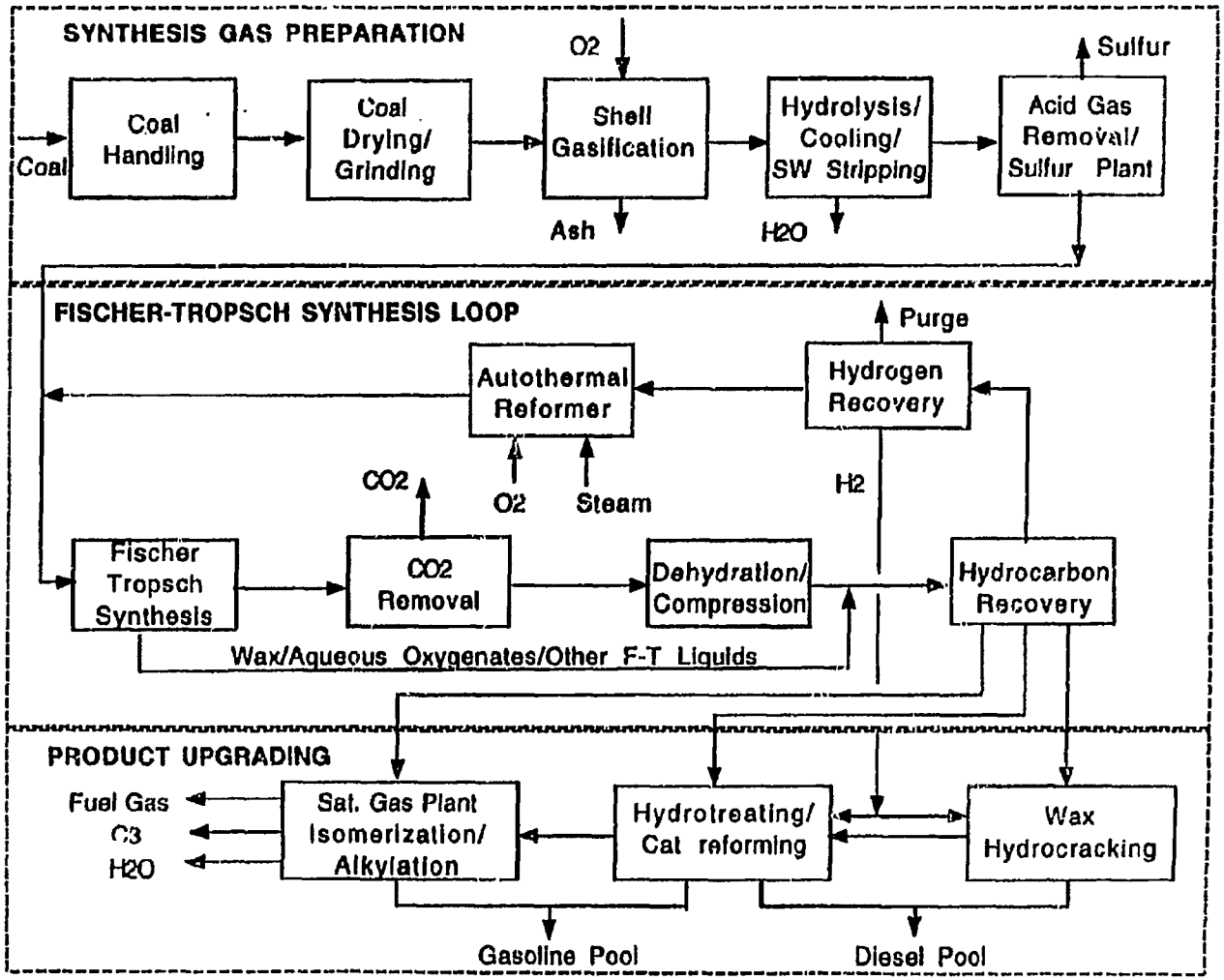


Figure 3-2

ASPEN BLOCK FLOW DIAGRAM FOR ILLINOIS COAL
AREA 100 - SYNGAS PRODUCTION

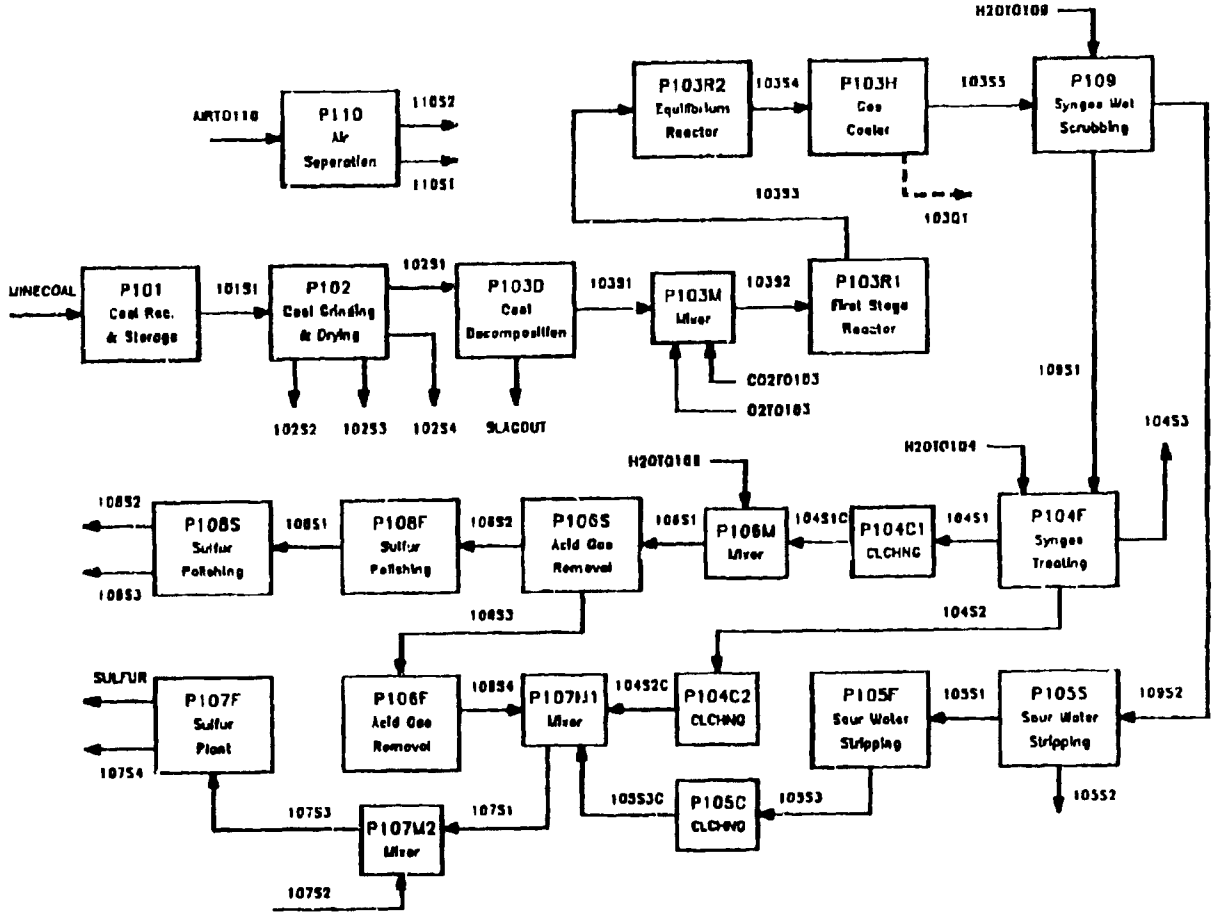


Figure 3-3

ASPEN BLOCK FLOW DIAGRAM FOR AREA 200 FISCHER-TROPSCH LOOP

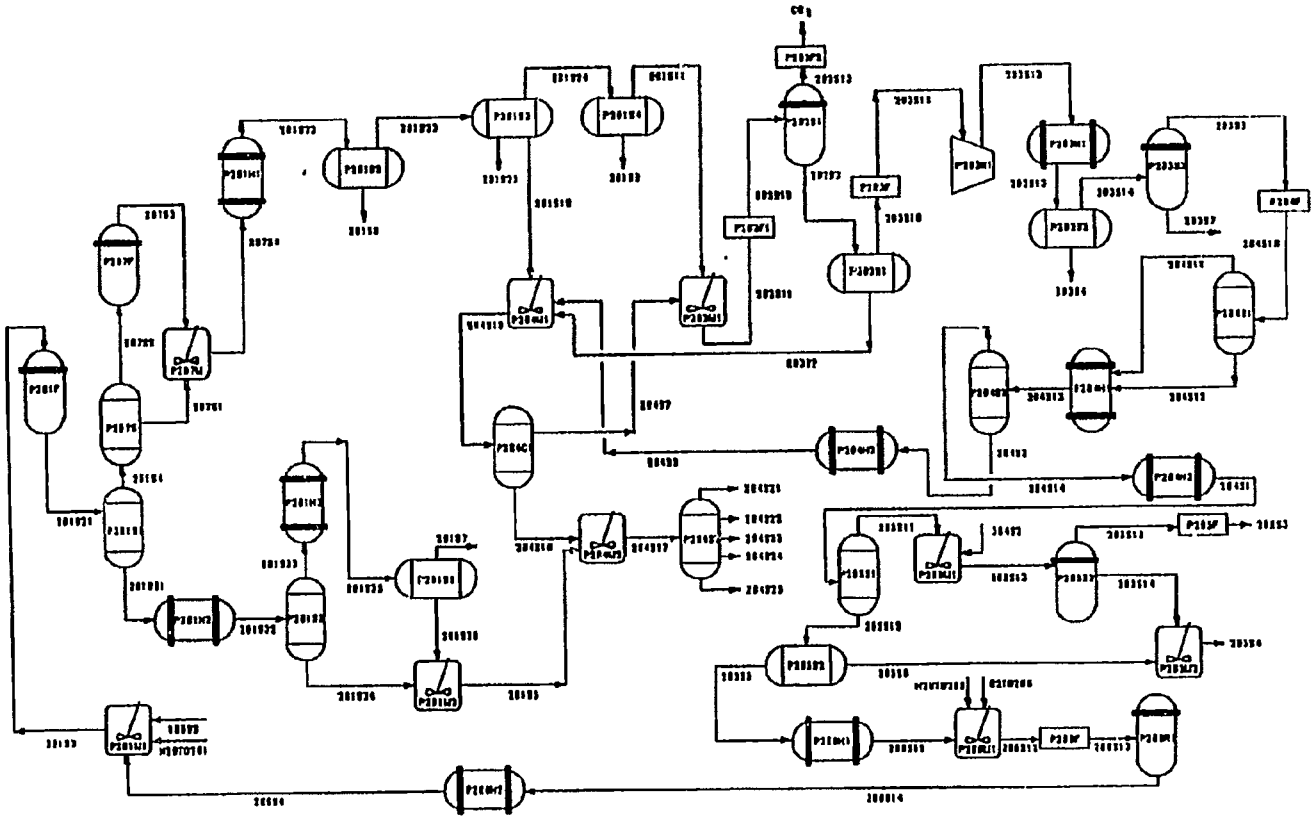


Figure 3-4

ASPEN BLOCK FLOW DIAGRAM FOR AREA 300
CONVENTIONAL REFINING CASE

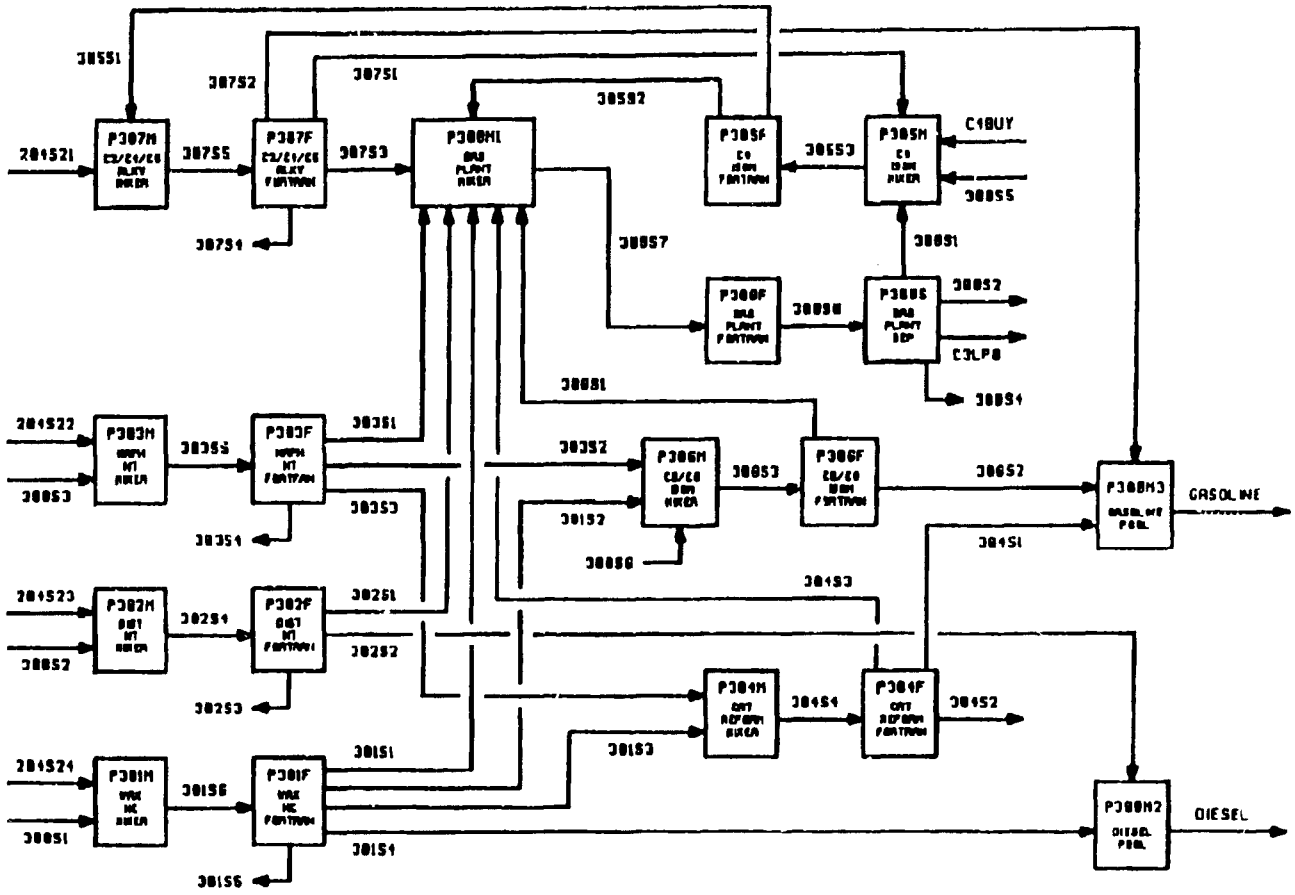


Figure 3-5

MANAGEMENT SUMMARY REPORT

MAJOR INPUT AND OUTPUT STREAMS

INPUT	MLBS/HR	TONS/DAY	
ROM COAL*	1547.933	18575.	
NATURAL GAS, MM SCF/HR			.000
ELECTRIC POWER, MEGA-WH/SD			1198.371
RAW WATER MAKE-UP, MM GAL/SD			14.460

OUTPUT	MLBS/HR	TONS/DAY	BBL/DAY
PROPANE	14.241	171.	1923.
BUTANES	-26.514	-318.	-3121.
GASOLINE	251.845	3022.	23952.
DIESEL	278.500	3342.	24681.
REFUSE*	.000	0.	
SLAG*	187.033	2244.	
SULFUR	46.689	560.	
TOTAL	751.794	9022.	47436.

* THESE STREAM FLOW RATES ARE ON A DRY BASIS.
NEGATIVE PRODUCT FLOWS DESIGNATE PURCHASED MATERIAL.

ISBL FIELD AND TOTAL INSTALLED COSTS (INCLUDING OSBL COSTS)

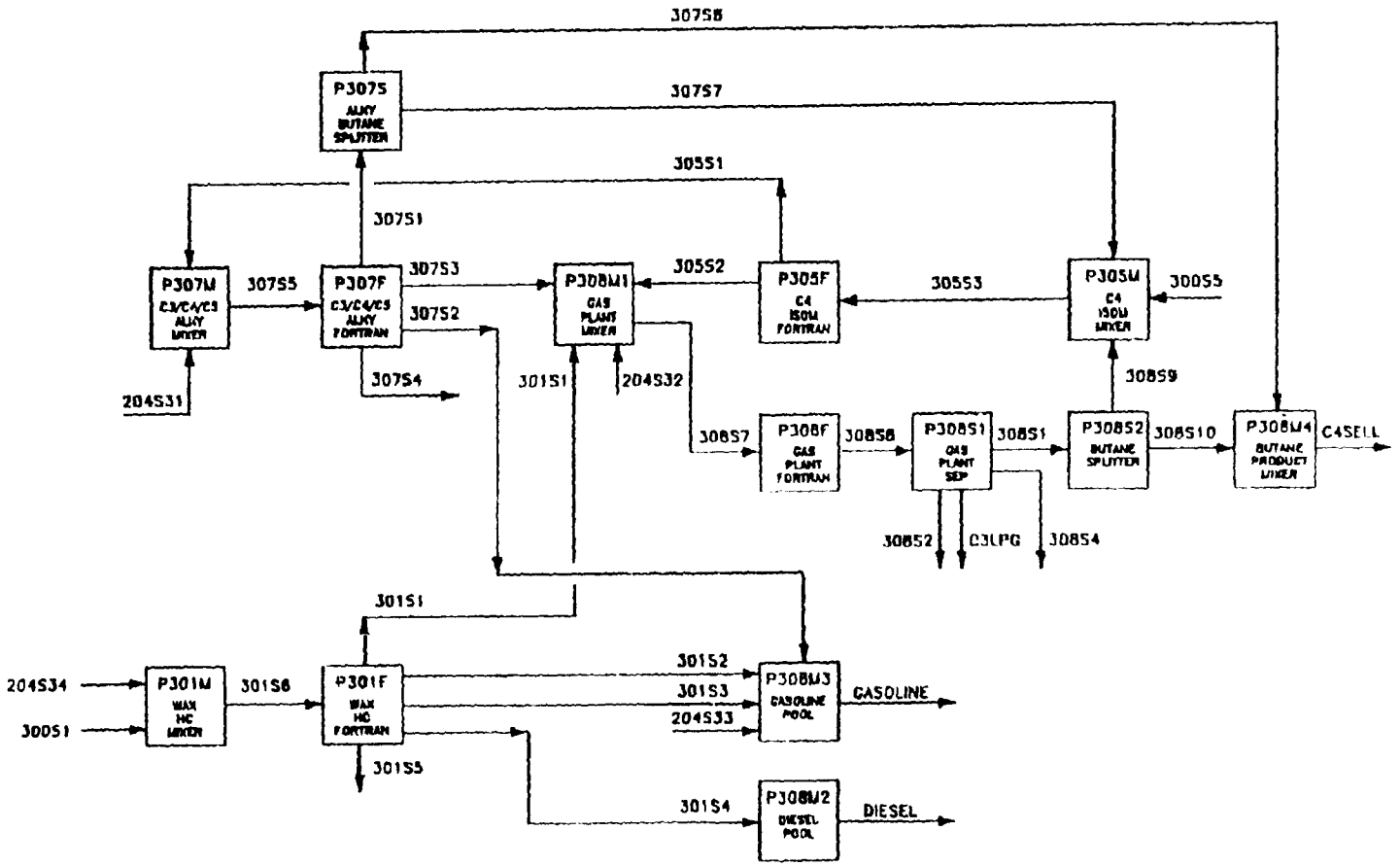
	NUMBER OF PLANTS		PLANT COST, MM$,		DEDICATED
PLANT	OPERATING	SPARES	ISBL	TOTAL	OPERATORS
101	1	0	42.020	63.862	12
102	5	1	101.220	153.833	17
103	8	1	702.910	1068.277	183
104	8	0	38.000	57.752	8
105	1	0	3.220	4.894	0
106	4	0	18.660	28.359	9
107	2	1	43.340	65.868	13
108	8	0	23.710	36.034	0
109	8	0	7.580	11.520	8
110	8	0	326.769	496.620	8
201	8	0	173.693	263.977	43
202A	8	0	16.795	25.523	0
202B	8	0	124.673	189.478	8
203	4	0	17.836	27.106	4
204	4	0	53.659	81.550	4
205	4	0	44.358	67.415	4
206	4	0	21.896	33.277	4
301	1	0	43.508	66.124	10
302	1	0	14.029	21.322	4
303	1	0	6.589	10.014	4
304	1	0	31.358	47.657	10
305	1	0	6.708	10.195	4
306	1	0	7.249	11.017	4
307	1	0	37.090	56.369	10
308	1	0	5.598	8.508	4
TOTAL			1912.468	2906.553	375

CATALYST AND CHEMICALS, MM$/YEAR	31.070

DEDICATED PLANT OPERATORS	375
EXTRA OPERATORS, FOREMEN AND MAINTENANCE WORKERS	713
TOTAL	1088

Figure 3-6

ASPEN BLOCK FLOW DIAGRAM FOR AREA 300
ALTERNATE REFINING CASE



Section 4

Project Management & Staffing Report

4.1 TASK 7 - PROJECT MANAGEMENT

During this reporting period, cost and schedule control was the primary activity. A technical paper entitled "Baseline Design/Economics for Advanced Fischer-Tropsch Technology" was presented in the DOE/PETC's Annual Contractors Review Conference, held at Pittsburgh, Pennsylvania, on September 27-29, 1993. A contract amendment was submitted to include the Kerr McGee ROSE unit in the Baseline design case and to convert the PFS models from the ASPEN/SP to ASPEN/Plus software code.

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	60
Samuel S. Tam	Project Manager	31
Gerald N. Choi	Process Engineer	90
Amoco		
R.D. Kaplan	Subcontract Manager	1
S. S. Kramer	Process Model/Simulation	85

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

Figure 4-1

Overall Milestone Schedule

(as of September 12, 1993)

PLAN STATUS REPORT

1. TITLE	2. REPORTING PERIOD	3. IDENTIFICATION NUMBER
Baseline Design/Economics for Advanced Fischer-Tropsch Technology	8/22/93 to 9/12/93	DE-AC22-91PC90027

4. PARTICIPANT NAME AND ADDRESS	5. START DATE	9/26/91
Bechtel Corporation 50 Beale Street San Francisco, CA 94105	6. COMPLETION DATE	9/25/93

7. ELEMENT CODE	8. REPORTING ELEMENT	9. DURATION FY 92 O N D J F M A M J J A S / FY 93 O N D J F M A M J J A S	10. PERCENT COMPLETE a. Plan	b. Actual
Task 1	Baseline Design		99	98
Task 2	Economic Evaluation		100	87
Task 3	Engineering Design Criteria		100	100
Task 4	Process Flowsheet Simulation Model		105	59
Task 5	Sensitivity Studies		100	27
Task 6	Documentation and Training			
Task 7	Project Management & Administration		97	82

△ Completion
① ASPEN/SP software delivered
② First progress meeting
③ Second progress meeting

① Baseline case design complete
② Baseline case equipment list transmitted to Cost Estimating

11. SIGNATURE OF PARTICIPANT'S PROJECT MANAGER AND DATE Samuel S. Tam 3/16/94

U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161 (703) 605-6000