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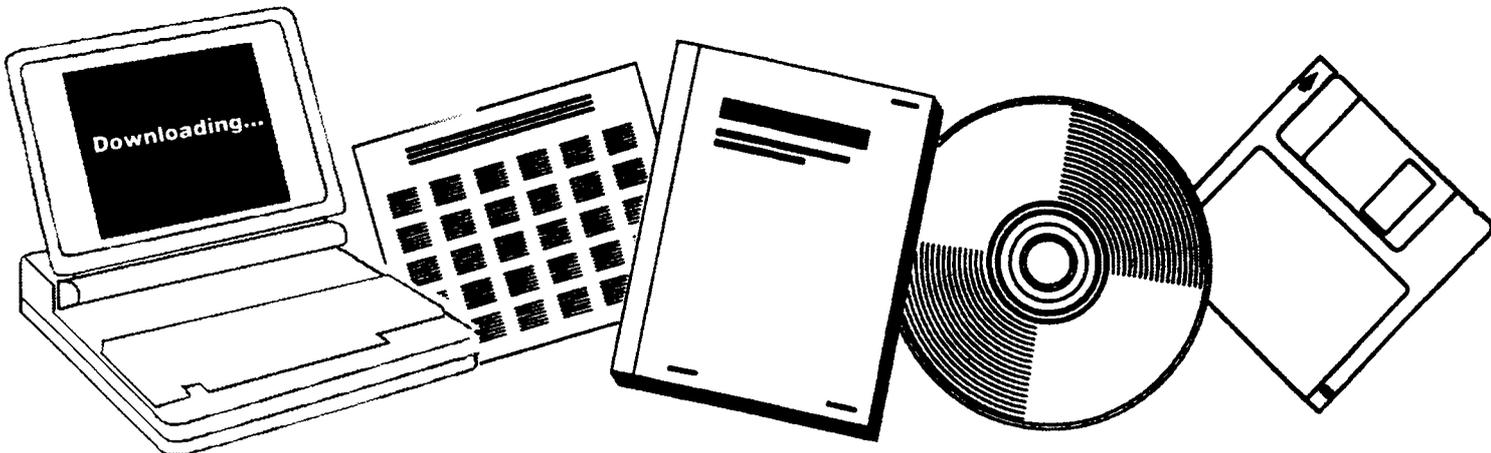
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**BASELINE DESIGN/ECONOMICS FOR ADVANCED  
FISCHER-TROPSCH TECHNOLOGY. QUARTERLY  
REPORT, JANUARY--MARCH 1994**

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

1994

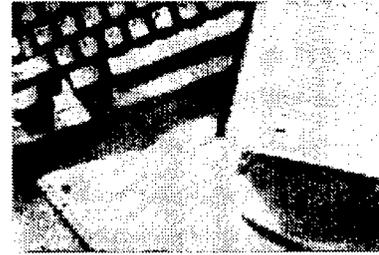


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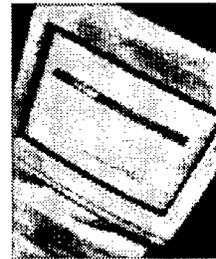
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**U.S. Department of Energy  
Pittsburgh Energy Technology Center**

**Baseline Design/Economics  
for  
Advanced Fischer-Tropsch Technology**

Contract No. DE-AC22-91PC90027

**Quarterly Report**

MAY 15 1995

OSTI

**October – December 1993**



We have no objection from a patent standpoint to the publication or dissemination of this material.

Mark Droschak 4/25/95  
Office of Intellectual Property Counsel Date  
DOE Field Office, Chicago

DOE/PC/90027--T9



**U.S. Department of Energy  
Pittsburgh Energy Technology Center**

**Baseline Design/Economics  
for  
Advanced Fischer-Tropsch Technology**

Contract No. DE-AC22-91PC90027

**Quarterly Report  
January – March 1994**



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## Section 1

# Introduction and Summary

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This report is Bechtel's tenth quarterly technical progress report and covers the period of January through March, 1994.

## 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 baseline design and computer model 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:

- o 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, 2, 4, 6 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 2 - Evaluate baseline and alternative economics.
- o Task 4 - Process Flowsheet Simulation (PFS) Model.
- o Task 6 - Document the PFS model and develop a DOE training session on its use.
- o Project Management and Staffing Report.

Completed work on Task 1, during the period of this report, consisted primarily of finalizing and reporting the Western Coal Case design. A Topical Report was prepared, summarizing the design basis and considerations, material and utility balances, capital and operating cost estimates. A similar report was written for the Alternate (ZSM-5) Refining Case reported earlier.

Under Task 2, preliminary economic analyses were performed on both the Alternate Refining Case and the Western Coal Case. Results were compared with each other and with that of the Baseline design. The same set of economic assumptions, taken directly from the Direct Liquefaction Baseline Study, as specified in the original Request of Work, was used for the analysis. This information was presented and discussed in the February 2, 1994 Technical Progress Meeting.

Under Tasks 4 and 6, some of the individual plant simulation models were further revised and enhanced. The three complete process simulation models were tuned to the latest utility balances and cost estimates, and the models were tested to verify that they were operable over the required ranges. A Topical Report, documenting the ASPEN process simulation models was drafted.

Under Task 7, cost and schedule control was the primary activity. A technical progress meeting was held at Bechtel San Francisco office, on February 2, 1994.

## Section 2

# **Task 1 - Baseline Design and Alternatives**

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Work progressed during this quarter consisted mainly of finalizing the Western Coal Case design. A Topical Report was drafted, documenting the design basis and considerations, material and utility balances, capital and operating cost estimates.

## **2.1 WESTERN COAL CASE**

Area 100 (Syngas Production) plant PFDs and process descriptions, along with material balance tables were reported in the fifth (October-December '92) Quarterly Report. Description of the Western Coal Case zero-discharge raw water treatment plant was presented in the last quarterly report (October-December '93).

Of the remaining design information, material balance summaries for Areas 200 and 300 are given in Tables 2-1 to 2-7, along with the overall plant utility summary (Table 2-8), steam flow distribution (Figure 2-1), and catalyst and chemical requirements, Table 2-9.

As a result of the February 2, 1994 technical progress review meeting, a new Fischer-Tropsch catalyst/wax separation scheme using Kerr McGee's Critical Solvent Extraction (ROSE) unit will be developed and incorporated into the baseline design. The Alternative Upgrading and Western Coal Case design will be revised as appropriate.

**Table 2-1**  
**Material Balance Summary**  
**Plant W201-Fischer Tropsch Synthesis**  
**(Wyoming Coal)**

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	Wax	Aqueous Oxygenates	Off Gas To Fuel
Phase	Vap	Liq	Vap	Vap	Liq	Liq	Vap
<b>Component Flows</b>							
<b>LBmol/hr</b>							
H2	36,553.00		48,926.00	14,439.00	0.64	0.00	3.42
N2	742.68		2,150.16	2,149.58	0.09		0.49
O2							
CO	89,801.00		96,990.00	11,780.00	0.51	0.00	2.77
CO2	6,195.78		7,952.02	53,747.00	10.25	3.34	23.67
H2O		4,610.32	9,555.39	2,607.01	3.55	2,205.05	1.99
CH4	23.29		416.34	1,368.12	0.13	0.00	0.46
C2H4			0.01	389.11	0.09		0.18
C2H6			0.01	97.28	0.03		0.05
C3H6				345.05	0.20		0.22
C3H8				60.89	0.04		0.04
IC4H8				13.46	0.02		0.01
NC4H8				255.63	0.30		0.20
IC4H10				3.36	0.00		0.00
NC4H10				63.90	0.08		0.05
C5H10				209.00	0.40		0.17
IC5H12				6.96	0.01		0.01
NC5H12				62.68	0.15		0.05
C6H12				173.20	0.67		0.12
IC6H14				5.77	0.02		0.00
NC6H14				51.94	0.22		0.03
C7-C19				975.99	52.64		0.12
WAX				3.04	453.69		
OXVAP				43.10	0.10	0.38	0.03
OXHC				163.51	1.48		0.02
OXH2O				167.96	0.36	157.96	0.09
Catalyst							
<b>Total</b>	133,315.75	4,610.32	165,989.94	89,172.53	525.66	2,366.73	34.18
<b>Total lb/hr</b>	2,882,900	83,056	3,404,400	3,111,000	292,120	47,087	1,264
<b>Mol. Wt.</b>	21.62	18.02	20.51	34.89	555.72	19.90	36.97
<b>MMSCFD</b>	1,214.24		1,511.84	812.18			

**Table 2-1 (Cont.)**  
**Material Balance Summary**  
**Plant W201-Fischer Tropsch Synthesis**  
**(Wyoming 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 Syngas	Pretreated Catalyst To F-T	Waste Catalyst To Disposal
Phase	Liq	Liq	Liq	vap	Slurry	Solid
Component Flows LBmol/hr						
H2		0.15	5.85	14,433.00		
N2			1.33	2,148.24		
O2						
CO		0.05	7.95	11,772.00		
CO2		0.00	345.15	53,399.00		
H2O	1,200.00	1,200.00	44.49	357.51		
CH4		0.00	2.39	1,365.73		
C2H4			2.31	386.79		
C2H6			0.82	96.45		
C3H6			7.72	337.33		
C3H8			1.56	59.33		
IC4H8			0.84	12.62		
NC4H8			16.22	239.40		
IC4H10			0.18	3.18		
NC4H10			4.68	59.22		
C5H10			31.12	177.88		
IC5H12			1.06	6.90		
NC5H12			11.76	50.92		
C6H12			61.41	111.79		
IC6H14			1.89	3.88		
NC6H14			20.38	31.56		
C7-C19			859.61	116.57		
WAX			3.04		1652.25'	24.25'
OXYAP		27.11	15.60			
OXHC			146.06	17.45		
OXH2O Catalyst					479.75'	479.75'
<b>Total</b>	<b>1,200.00</b>	<b>1,227.32</b>	<b>1,593.43</b>	<b>85,185.77</b>		
<b>Total lb/hr</b>	<b>21,618</b>	<b>23,000</b>	<b>173,750</b>	<b>2,888,800</b>	<b>2132</b>	<b>504</b>
<b>Mol. Wt.</b>	<b>18.02</b>	<b>18.74</b>	<b>109.04</b>	<b>33.91</b>		
<b>MMSCFD</b>				<b>775.87</b>		

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

**Table 2-2**  
**Material Balance Summary**  
**Plant W202-CO2 Removal**  
**(Wyoming Coal)**

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	14,433.00	19.17	14,452.00	
N2	2,148.24	13.54	2,161.85	
O2				
CO	11,772.00	89.62	11,861.00	
CO2	53,399.00	500.65	269.50	53,630.00
H2O	357.51	0.00	357.52	
CH4	1,365.73	58.07	1,423.80	
C2H4	386.79	256.12	642.90	
C2H6	96.45	124.58	221.02	
C3H6	337.33	16.91	354.24	
C3H8	59.33	1.78	61.11	
IC4H8	12.62		12.62	
NC4H8	239.40		239.40	
IC4H10	3.18		3.18	
NC4H10	59.22		59.22	
C5H10	177.88		177.88	
IC5H12	5.90		5.90	
NC5H12	50.92		50.92	
C6H12	111.79		111.79	
IC6H14	3.88		3.88	
NC6H14	31.56		31.57	
C7-C19	116.57		116.57	
WAX				
OXVAP				
OXHC	17.45		17.45	
OXH2O				
<b>Total</b>	<b>85,185.77</b>	<b>1,080.43</b>	<b>32,635.33</b>	<b>53,630.00</b>
<b>Total lb/hr</b>	<b>2,888,800</b>	<b>37,614</b>	<b>566,150</b>	<b>2,360,200</b>
<b>Mol.Wt</b>	<b>33.91</b>	<b>34.81</b>	<b>17.35</b>	<b>44.01</b>
<b>MMSCFD</b>	<b>775.87</b>	<b>9.84</b>	<b>297.24</b>	<b>488.46</b>

**Table 2-3**  
**Material Balance Summary**  
**Plant W203-Compression & Dehydration**  
**(Wyoming Coal)**

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	14,452.00	0.66	14,452.00		1,795.70	2265.14	4060.84
N2	2,161.85	0.15	2,161.70		330.11	416.41	746.52
O2							
CO	11,861.00	0.93	11,860.00		1,808.90	2281.79	4090.69
CO2	269.50	0.25	269.25		17.04	21.50	38.54
H2O	357.52	8.84		259.57			89.31
CH4	1,423.80	0.32	1,423.48		240.93	303.92	544.85
C2H4	642.90	0.53	642.37		59.59	75.17	134.77
C2H6	221.02	0.27	220.76		58.63	73.96	132.59
C3H6	354.24	1.22	353.02		3.66	4.62	8.28
C3H8	61.11	0.24	60.87		0.50	0.63	1.13
IC4H8	12.62	0.13	12.49		0.01	0.02	0.03
NC4H8	239.40	2.55	236.85		0.24	0.31	0.55
IC4H10	3.18	0.03	3.15		0.01	0.01	0.01
NC4H10	59.22	0.73	58.49		0.04	0.06	0.10
C5H10	177.88	5.16	172.72		0.02	0.02	0.04
IC5H12	5.90	0.17	5.73				0.00
NC5H12	50.92	1.88	49.04		0.00	0.00	0.01
C6H12	111.79	9.73	102.06				0.00
IC6H14	3.88	0.30	3.59				
NC6H14	31.57	3.15	28.42				
C7-C19	116.57	41.72	74.84				
WAX							
OXVAP							
OXHC	17.45	11.51	5.95				
OXH2O							
<b>Total</b>	<b>32,635.33</b>	<b>90.26</b>	<b>32,196.79</b>	<b>259.57</b>	<b>4,315.41</b>	<b>5,443.54</b>	<b>9,848.26</b>
<b>Total lb/hr</b>	<b>566,150</b>	<b>7,840</b>	<b>552,030</b>	<b>4,676</b>	<b>71,782</b>	<b>90,540</b>	<b>163,939</b>
<b>Mol. Wt.</b>	<b>17.35</b>	<b>86.88</b>	<b>17.15</b>	<b>18.02</b>	<b>16.63</b>	<b>16.63</b>	<b>16.65</b>
<b>MMSCFD</b>	<b>297.24</b>		<b>293.25</b>		<b>39.30</b>	<b>49.58</b>	<b>89.70</b>

**Table 2-4**  
**Material Balance Summary**  
**Plant W204-Hydrocarbon Recovery**  
**(Wyoming Coal)**

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	14,439.00	14,452.00	12.66	0.66	5.85		19.17
N2	2,149.64	2,161.70	12.05	0.15	1.33		13.54
O2							
CO	11,779.00	11,860.00	80.74	0.93	7.95		89.62
CO2	110.97	269.25	158.27	0.25	345.15	3.02	500.65
H2O				8.64	44.49	53.12	
CH4	1,368.12	1,423.49	55.36	0.32	2.39		58.07
C2H4	388.07	642.37	254.30	0.53	2.31	1.03	256.12
C2H6	90.99	220.76	129.77	0.27	0.82	6.28	124.58
C3H6	23.84	353.02	329.18	1.22	7.72	321.21	16.91
C3H8	3.26	60.87	57.62	0.24	1.56	57.63	1.78
IC4H8	0.09	12.49	12.41	0.13	0.84		13.37
NC4H8	1.59	236.85	235.26	2.55	16.22	254.04	
IC4H10	0.03	3.15	3.12	0.03	0.18	3.33	
NC4H10	0.29	58.49	58.20	0.73	4.68	63.61	
C5H10	0.11	172.72	172.61	5.16	31.12	208.89	
IC5H12	0.00	6.73	6.73	0.17	1.06	6.96	
NC5H12	0.02	49.04	49.02	1.88	11.76	62.66	
C6H12	0.01	102.06	102.05	9.73	61.41	173.19	
IC6H14		3.59	3.59	0.30	1.89	5.77	
NC6H14	0.00	28.42	28.41	3.15	20.38	51.94	
C7-C19		74.84	74.84	41.72	859.61	976.18	
WAX					3.04	3.04	
OXVAP					15.60	15.60	
OXHC		5.95	5.95	11.51	146.06	163.51	
OXH2O							
<b>Total</b>	<b>30,355.05</b>	<b>32,196.79</b>	<b>1,841.13</b>	<b>90.26</b>	<b>1,593.43</b>	<b>2,444.39</b>	<b>1,080.43</b>
<b>Total lb/hr</b>	<b>461,000</b>	<b>552,030</b>	<b>91,030</b>	<b>7,840</b>	<b>173,750</b>	<b>235,010</b>	<b>37,614</b>
<b>Mol. Wt.</b>	<b>15.19</b>	<b>17.15</b>	<b>49.44</b>	<b>86.86</b>	<b>109.04</b>	<b>96.14</b>	<b>34.81</b>
<b>MMSCFD</b>	<b>276.47</b>	<b>293.25</b>					<b>9.84</b>

**Table 2-4 (Cont.)**  
**Material Balance Summary**  
**Plant W204-Hydrocarbon Recovery**  
**(Wyoming Coal)**

Stream No.	204.12	204.13	204.14	204.15	204.16	204.19
	Feed To Product Fractionator	Fractionator Overhead To Alkylation	Condensate To water Treatment	Naphtha To Hydrotreating Plant	Distillate To Hydrotreating Plant	Wax To Hydrocracking Plant
Phase	Liq	Vap	Liq	Liq	Liq	Liq
<b>Component Flows</b>						
<b>Lbmol/hr</b>						
H2	0.64	0.64				
N2	0.09	0.09				
O2						
CO	0.51	0.51				
CO2	13.27	10.62	2.65			
H2O	56.68	8.50	48.18			
CH4	0.13	0.13				
C2H4	1.12	1.12				
C2H6	6.31	6.31				
C3H6	321.41	321.41				
C3H8	57.67	57.67				
IC4H8	13.39	13.39				
NC4H8	254.33	254.33				
IC4H10	3.33	3.33				
NC4H10	63.69	63.69				
C5H10	209.30	209.76		0.54		
IC5H12	6.97	6.97		0.00		
NC5H12	62.81	22.58		40.22		
C6H12	173.86			173.86		
IC6H14	5.80			5.80		
NC6H14	52.16			52.16		
C7-C19	1,028.82			594.01	434.81	
WAX	456.73					456.73
OXVAP						
OXHC	164.99			79.19	85.79	
OXH2O						
<b>Total</b>	<b>2,953.09</b>	<b>980.05</b>	<b>50.83</b>	<b>945.78</b>	<b>520.60</b>	<b>456.73</b>
<b>Total lb/hr</b>	<b>526,314</b>	<b>52,820</b>	<b>985</b>	<b>98,654</b>	<b>91,879</b>	<b>282,170</b>
<b>Mol. Wt.</b>	<b>178.17</b>	<b>53.69</b>	<b>19.37</b>	<b>104.31</b>	<b>176.49</b>	<b>617.81</b>
<b>NMSCFD</b>		<b>8.93</b>				

**Table 2-5**  
**Material Balance Summary**  
**Plant W205-Hydrogen Recovery**  
**(Wyoming Coal)**

Stream No.	205.1	205.2	205.3	205.4	205.5
	H2 From Cat. Reformer Area 300	Recycle Gas From Plant 204	H2 Product From PSA	Fuel (Purge) Gas	Autothermal Reformer Feed
Phase	Vap	Vap	Vap	Vap	Vap
<b>Component Flows</b>					
Lbmol/hr					
H2	2,113.03	14,439.00	3,066.51	4,060.84	9,424.75
N2		2,149.64		746.52	1,403.13
O2					
CO		11,779.00		4,090.69	7,688.69
CO2		110.97		38.54	72.44
H2O					
CH4	69.73	1,368.12		544.85	893.01
C2H4		388.07		134.77	253.30
C2H6	100.99	90.99		132.59	59.39
C3H6		23.84		8.28	15.56
C3H8		3.26		1.13	2.13
IC4H8		0.09		0.03	0.06
NC4H8		1.59		0.55	1.04
IC4H10		0.03		0.01	0.02
NC4H10		0.29		0.10	0.19
C5H10		0.11		0.04	0.07
IC5H12		0.00		0.00	0.00
NC5H12		0.02		0.01	0.01
C6H12		0.01		0.00	0.00
IC6H14		0.00			
NC6H14		0.00			0.00
C7-C19					
WAX					
OXVAP					
OXHC					
OXH2O					
<b>Total</b>	<b>2,283.75</b>	<b>30,355.05</b>	<b>3,066.51</b>	<b>9,758.95</b>	<b>19,813.89</b>
<b>Total lb/hr</b>	<b>8,415</b>	<b>461,000</b>	<b>6,181</b>	<b>162,330</b>	<b>300,900</b>
<b>Mol. Wt.</b>	<b>3.68</b>	<b>15.19</b>	<b>2.02</b>	<b>16.63</b>	<b>15.19</b>
<b>MMSCFD</b>	<b>20.80</b>	<b>276.47</b>	<b>27.93</b>	<b>88.88</b>	<b>180.46</b>

**Table 2-6**  
**Material Balance Summary**  
**Plant W206-Autothermal Reformer**  
**(Wyoming Coal)**

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
<b>Component Flows</b>				
Lbmol/hr				
H2			9,424.75	12,373.00
N2	4.36		1,403.13	1,407.48
O2	832.51			
CO			7,688.69	7,188.96
CO2			72.44	1,756.24
H2O		6,147.93		4,945.06
CH4			893.01	393.05
C2H4			253.30	0.01
C2H6			59.39	0.01
C3H6			15.56	
C3H8			2.13	
IC4H8			0.06	
NC4H8			1.04	
IC4H10			0.02	
NC4H10			0.19	
C5H10			0.07	
IC5H12			0.00	
NC5H12			0.01	
C6H12			0.00	
IC6H14				
NC6H14			0.00	
C7-C19				
WAX				
OXVAP				
OXHC				
OXH2O				
<b>Total</b>	<b>836.86</b>	<b>6,147.93</b>	<b>19,813.80</b>	<b>28,063.83</b>
<b>Total lb/hr</b>	<b>26,761</b>	<b>110,760</b>	<b>300,900</b>	<b>438,420</b>
<b>Mol. Wt.</b>	<b>31.98</b>	<b>18.02</b>	<b>15.19</b>	<b>15.62</b>
<b>MMSCFD</b>	<b>7.62</b>	<b>56.00</b>	<b>180.46</b>	<b>255.61</b>

**Table 2-7 (1)**  
**Material Balance Summary**  
**Area W300 -Product Upgrading and Refining Summary**  
**(Wyoming Coal)**

Component	Naphtha Hydrotreating						Distillate Hydrotreating			
	Feed	H2 Required	C4-	C5/C6	C7+ Naphtha	H2O Prodced	Feed	H2 Required	C4-	Diesel
	204.2	300.3	303.1	303.2	303.3	303.4	204.16	300.2	302.1	302.2
H2		1471	0	0	0			726	0	0
N2	0		0	0	0		0		0	0
O2	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		358	0	0		0		84	0
C2=	0		0	0	0		0		0	0
C2	0		1378	0	0		0		127	0
C3=	0		0	0	0		0		0	0
C3	0		1752	0	0		0		296	0
IC4	0		243	0	0		0		127	0
nC4	0		1171	0	0		0		211	0
C4=	0		0	0	0		0		0	0
IC5	25		0	78	0		0		0	0
nC5	3625		0	4207	0		0		0	0
C5=	0		0	0	0		0		0	0
C6=	14632		0	0	0		0		0	0
IC6	499		0	2000	0		0		0	0
nC6	4495		0	17906	0		0		0	0
C7-C10 (Naphtha)	69258		0	0	0		0		0	0
C11-C19 (Distillate)	0		0	0	0		84400		0	0
C19+ (Wax)	0		0	0	0		0		0	0
180-300OX	6960		0	0	0		0		0	0
300-350OX	730		0	0	0		0		0	0
350-700OX	0		0	0	0		6528		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	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	54500		0		0	0
300-350 HTU	0		0	0	15471		0		0	0
350-500 HTU	0		0	0	0		0		0	54305
500+ HTU	0		0	0	0		0		0	35751
H2O Produced	0		0	0	0	2437	0		0	0
<b>Total (Lb/hr)</b>	<b>100225</b>	<b>1471</b>	<b>4902</b>	<b>24361</b>	<b>69971</b>	<b>2437</b>	<b>91008</b>	<b>726</b>	<b>845</b>	<b>90056</b>
<b>Total (BPSD)</b>	<b>9545</b>			<b>2545</b>	<b>6758</b>	<b>167</b>	<b>8054</b>		<b>105</b>	<b>8093</b>
<b>Density (lb/ft3)</b>	<b>44.4110</b>		<b>31.2678</b>	<b>40.9151</b>	<b>44.2551</b>	<b>62.2978</b>	<b>48.2960</b>		<b>34.4807</b>	<b>47.5588</b>
<b>Mol. Wt</b>	<b>99.87</b>	<b>2.02</b>	<b>37.08</b>	<b>83.28</b>	<b>117.85</b>	<b>18.02</b>	<b>192.53</b>	<b>2.02</b>	<b>38.40</b>	<b>192.28</b>

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**Table 2-7 (2)**  
**Material Balance Summary**  
**Area W300 -Product Upgrading and Refining Summary**  
**(Wyoming Coal)**

Component	Wax Hydrocracking									
	H2O Produced	Feed	H2 Required	C4-	C5/C6's	C7, Naphtha	Distillate	H2O Produced	Olain Feed	iC4 Makeup
	302.3	204.12	300.1	301.1	301.2	301.3	301.4	301.5	204.9+204.13	305.1
H2			3809	0	0	0	0		0	0
N2		0		0	0	0	0		0	0
O2		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		139	0	0	0		0	0
C2-		0		0	0	0	0		0	0
C2		0		139	0	0	0		0	0
C3-		0		0	0	0	0		13525	0
C3		0		4148	0	0	0		2543	0
iC4		0		5494	0	0	0		194	46198
nC4		0		4457	0	0	0		3702	1924
C4-		0		0	0	0	0		15021	0
iC5		0		0	6638	0	0		478	0
nC5		0		0	5776	0	0		906	0
C5-		0		0	0	0	0		14679	0
C6-		0		0	0	0	0		0	0
iC6		0		0	10875	0	0		0	0
nC6		0		0	6670	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)		282174		0	0	0	0		0	0
180-300OX		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		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 Isomate		0		0	0	0	0		0	0
C6 Isomate		0		0	0	0	0		0	0
C7-300 HC		0		0	0	40588	0		0	0
300-350 HC		0		0	0	13034	0		0	0
350-500 HC		0		0	0	0	59426		0	0
500-700 HC		0		0	0	0	126506		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
H2O Produced	833	0		0	0	0	0	1892	0	0
Total (Lb/hr)	833	282174	3809	14378	30159	53622	185932	1892	51049	48122
Total (BPSD)	57	20730			3205	5178	16365	130	6009	5060
Density (lb/ft3)	62.2978	58.1778			48.2197	44.2642	48.5581	62.2978	36.3062	35.1006
Mol. Wt	18.02	817.82	2.02	51.61	79.70			18.02	54.17	58.12

**Table 2-7 (3)**  
**Material Balance Summary**  
**Area W300 -Product Upgrading and Refining Summary**  
**(Wyoming Coal)**

Component	C3/C4/C5 Alkylation				C4 Isomerization			C5/C6 Isomerization		
	C4's 307.1	Alkylate 307.2	C3 307.3	HC Acid Loss 307.4	Purchased C4 300.4	H2 Required 300.5	Fuel Gas 305.2	C4 306.1	Isomrate 306.2	H2 Required 300.6
H2	0	0	0		0	22	0	0	0	78
N2	0	0	0		0		0	0	0	
OO	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	0	0		0		92	49	0	
C2=	0	0	0		0		0	0	0	
C2	0	0	0		0		207	16	0	
C3=	0	0	0		0		0	0	0	
C3	0	0	2543		0		559	644	0	
IC4	0	0	0		1323		0	300	0	
nC4	5626	0	0		25145		0	0	0	
C4=	0	0	0		0		0	0	0	
IC5	0	478	0		0		0	0	0	
nC5	0	906	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	
180-300OX	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	32216	0		0		0	0	0	
C4 Alkylate	0	30779	0		0		0	0	0	
C5 Alkylate	0	25682	0		0		0	0	0	
C5 isomrate	0	0	0		0		0	0	16680	
C6 isomrate	0	0	0		0		0	0	36899	
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	
H2O Produced	0	0	0	932	0		0	0	0	
Total (Lb/hr)	5626	90061	2543	932	28469	22	858	1010	53588	78
Total (BPSD)	661	8695			3115				5635	
Density (lb/ft3)	36.3878	44.2698	31.5859		36.3205		31.7323	34.0043	40.6473	
Mol. Wt	58.12	106.87	44.10		58.12	2.02	33.92	100.27	81.26	2.02

**Table 2-7 (4)**  
**Material Balance Summary**  
**Area W300 -Product Upgrading and Refining Summary (4)**  
**(Wyoming Coal)**

Component	Catalytic Reforming			Saturated Gas plant/Product Recovery					
	Reformate	H2/C2-	C3/C4	C4'S	C2- Fuel Gas	C3	H2O	Gasoline	Diesel
	304.1	304.2	304.3	308.1	308.2	308.3	308.4	308.5	308.6
H2	0	4254	0	0	1	0		0	0
N2	0	0	0	0	2	0		0	0
CO	0	0	0	0	14	0		0	0
CO2	0	0	0	0	467	0		0	0
H2O	0	0	0	0	0	0	153	0	0
C1	0	1117	0	0	725	0		0	0
C2-	0		0	0	31	0		0	0
C2	0	3033	0	0	2015	41		0	0
C3-	0		0	0	0	0		0	0
C3	0	0	3856	0	0	13798		0	0
IC4	0	0	2319	8313	0	170		0	0
nC4	0	0	2885	8550	0	174		0	0
C4-	0	0	0	0	0	0		0	0
IC5	0	0	0	0	0	0		478	0
nC5	0	0	0	0	0	0		808	0
C5-	0	0	0	0	0	0		0	0
C6-	0	0	0	0	0	0		0	0
IC6	0	0	0	0	0	0		0	0
nC6	0	0	0	0	0	0		0	0
C7-C10 (Naphtha)	0	0	0	0	0	0		0	0
C11-C19 (Distillate)	0	0	0	0	0	0		0	0
C19+ (Wax)	0	0	0	0	0	0		0	0
180-300OX	0	0	0	0	0	0		0	0
300-350OX	0	0	0	0	0	0		0	0
350-700OX	0	0	0	0	0	0		0	0
Reformate	106130	0	0	0	0	0		106130	0
C3 Alkylate	0	0	0	0	0	0		32216	0
C4 Alkylate	0	0	0	0	0	0		30779	0
C5 Alkylate	0	0	0	0	0	0		25682	0
C5 Isomerate	0	0	0	0	0	0		16688	0
C6 Isomerate	0	0	0	0	0	0		38899	0
C7-300 HC	0	0	0	0	0	0		0	0
300-350 HC	0	0	0	0	0	0		0	0
350-500 HC	0	0	0	0	0	0		0	59426
500-700 HC	0	0	0	0	0	0		0	126506
C7-300 HTU	0	0	0	0	0	0		0	0
300-350 HTU	0	0	0	0	0	0		0	0
350-500 HTU	0	0	0	0	0	0		0	54305
500+ HTU	0	0	0	0	0	0		0	35751
H2O Produced	0	0	0	0	0	0		0	0
Total (Lb/hr)	106130	8404	9059	18864	3257	14183	153	249778	275988
Total (BPSD)	8428		1143	2018		1918	11	23758	24452
Density (lb/lb3)	48.1079		33.8653	38.7152		31.8356	62.2978	44.9339	48.2275
Mol. Wt		3.88	51.19	58.12	25.51	44.30	18.02		

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**Table 2-8 (1)**

**Western (Wyoming) Coal Design  
Utility Balance Summary**

Plant No.	Plant Description	Load BHP	Power kW	Steam, M lb/hr					
				900 Psig/1000 °F		600 Psig/650 °F		600 Psig/Sat'd	
				Produced	Consumed	Produced	Consumed	Produced	Consumed
	<b>Area 100</b>								
W101	Coal Receiving/Storage	2900	2403						
W102	Coal Drying/Grinding	40696	33732						
W103	Shell Gasification	66160	55134	2429		500			
W105	Sour Water Stripping	146	121						
W106	Acid Gas Removal	9050	7542						
W107	Sulfur Recovery/TGT	347	288					25	7
W108	Sulfur Polishing	0	0						
W109	Syngas Wet Scrubbing	792	660						
W110	Air Separation	458	381		2425				
	Subtotal:	120549	100261	2429	2425	500	0	25	7
	<b>Area 200</b>								
W201	F-T Synthesis	4894	4045				16		
W202	CO2 Removal	9595	7930						
W203	Dehydration/Compress	0	0				9		
W204	Hydrocarbon Recovery	1198	990				68		
W205	Hydrogen Recovery	16	12						
W206	Autothermal Reforming	0	0						122
	Subtotal:	15704	12977	0	0	0	93	0	122
	<b>Area 300</b>								
W301	Wax Hydrocracking	2479	1999				67		
W302	Distillate Hydrotreating	1365	1075						
W303	Naphtha Hydrotreating	947	746						
W304	Catalytic Reforming	3754	2956			22			
W305	C4 Isomerization	872	687				7		
W306	C5/C6 Isomerization	118	93				6		
W307	C3/C4/C5 Alkylation	8463	6664				17		
W308	Saturated Gas Plant	119	94				9		
	Subtotal:	18119	14314	0	0	22	106	0	0
	<b>Offsites</b>								
W19	Relief and Blowdown	23	19		4		323	104	
W20	Tankage	87	72						
W21	Intercon. Piping System	0	0						
W22	Product Shipping	1617	1270						
W23	Tank Car/Truck Loading	39	32						
W24	Coal Refuse/Ash Disposal	60	50						
W25	Cat./Chem. Handling	60	50						
W31	Steam and Power Gener.	-83921	-65900						
W32	Raw/Cooking/Pot. Water	10519	8260						
W33	Fire Protection System	53	44						
W34	Sewage/Effl. Treatment	6234	4895						
W35	Instrument/Plant Air	3685	2894						
W36	Purge/Plush Oil System	0	0						
W37	Solid Waste Management	59	49						
W40	General Site	0	0						
W41	Buildings	3428	2692						
W42	Telecommunications	16	13						
Other	Miscellaneous	2710	2128						
	Subtotal:	-55331	-43432	0	4	0	323	104	0
<b>TOTAL</b>		<b>99041</b>	<b>84120</b>	<b>2429</b>	<b>2429</b>	<b>522</b>	<b>522</b>	<b>129</b>	<b>129</b>

(-) indicates Production

**Table 2-8 (2)**  
**Western (Wyoming) Coal Design**  
**Utility Balance Summary**

Plant No.	Plant Description	Steam, M lb/hr				Steam, M lb/hr			
		360 Psig/600 ° F		360 Psig/Sa'd		150 Psig/Sa'd		50 Psig/Sa'd	
		Produced	Consumed	Produced	Consumed	Produced	Consumed	Produced	Consumed
<b>Area 100</b>									
W101	Coal Receiving/Storage								
W102	Coal Drying/Grinding				365			58	
W103	Shell Gasification								
W105	Sour Water Stripping								23
W106	Acid Gas Removal					24		2	104
W107	Sulfur Recovery/TGT							23	54
W108	Sulfur Polishing								
W109	Syngas Wet Scrubbing								
W110	Air Separation						15	819	
	Subtotal:	0	0	0	365	0	39	902	181
<b>Area 200</b>									
W201	F-T Synthesis			3273				4	
W202	CO2 Removal		443					443	3180
W203	Dehydration/Compress		247					249	
W204	Hydrocarbon Recovery		348		49			371	30
W205	Hydrogen Recovery		49					49	
W206	Autothermal Reforming							1	
	Subtotal:	0	1087	3273	49	0	0	1117	3210
<b>Area 300</b>									
W301	Wax Hydrocracking		209					224	30
W302	Distillate Hydrotreating							3	
W303	Naphtha Hydrotreating								
W304	Catalytic Reforming								
W305	C4 Isomerization					1		2	72
W306	C5/C6 Isomerization							1	
W307	C3/C4/C5 Alkylation							4	50
W308	Saturated Gas Plant							2	
	Subtotal:	0	209	0	0	0	1	236	152
<b>Offsites</b>									
W19	Relief and Blowdown			223	40	40			
W20	Tankage								
W21	Intercon. Piping System								
W22	Product Shipping								
W23	Tank Car/Truck Loading								
W24	Coal Refuse/Ash Disposal								
W25	Cat./Chem. Handling								
W31	Steam and Power Gener.	3042	1439		3042			1070	
W32	Raw/Cooling/Pot. Water		307					307	
W33	Fire Protection System								
W34	Sewage/Emf. Treatment								
W35	Instrument/Plant Air								
W36	Purge/Flush Oil System								
W37	Solid Waste Management								
W40	General Site								
W41	Buildings								
W42	Telecommunications								
Other	Miscellaneous								89
	Subtotal:	3042	1746	223	3082	40	0	1377	89
<b>TOTAL</b>		<b>3042</b>	<b>3042</b>	<b>3496</b>	<b>3496</b>	<b>40</b>	<b>40</b>	<b>3632</b>	<b>3632</b>

(-) indicates Production

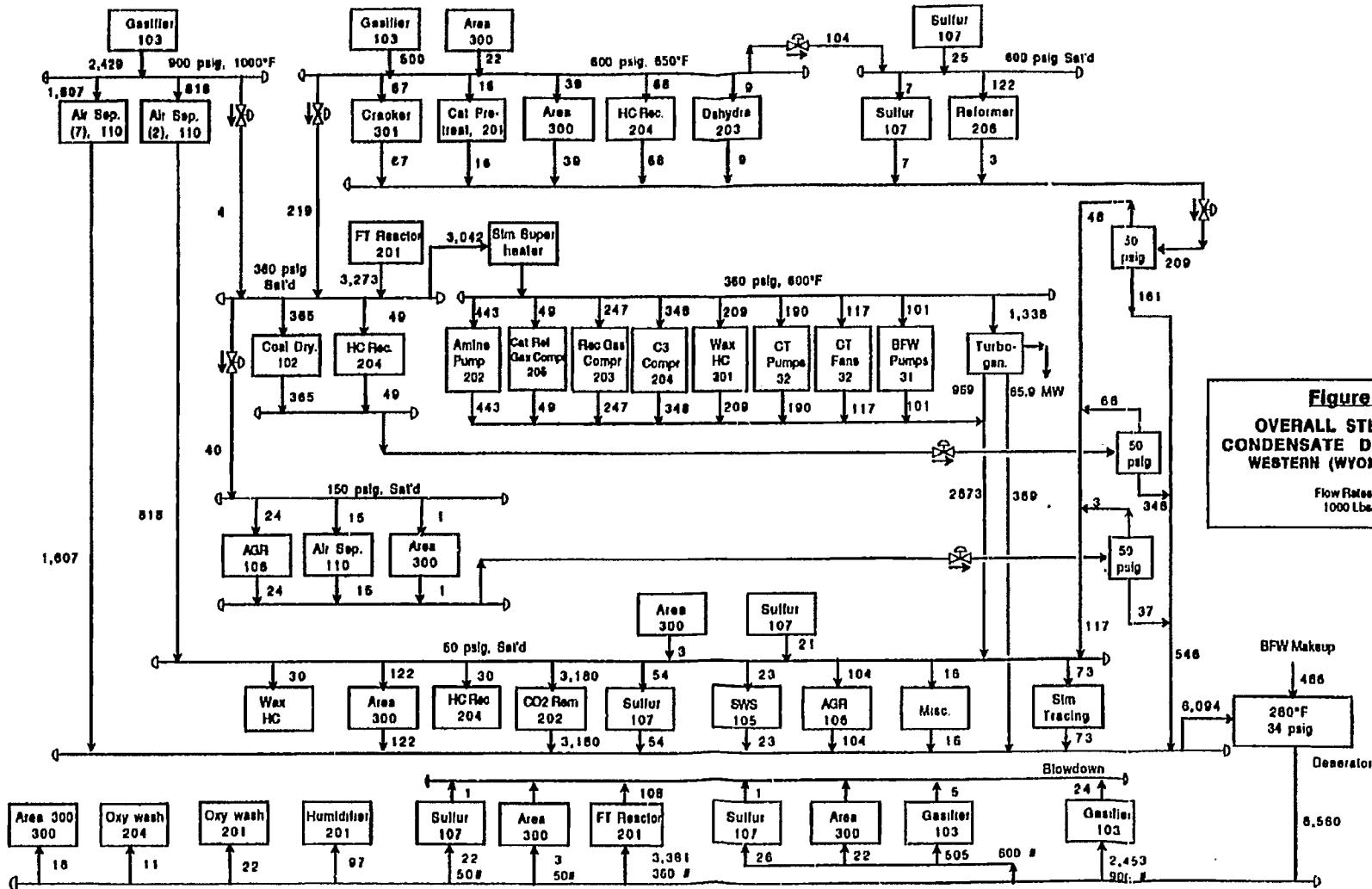
**Table 2-8 (3)**  
**Western (Wyoming) Coal Design**  
**Utility Balance Summary**

Plant No.	Plant Description	Condensate Mlb/hr	BFW Mlb/hr	Water Process Mlb/hr	C.W. Circ. GPM	Cooling, MMBtu/hr		Fuel, MMBtu/hr Total Fired
						Air	Water	
	<b>Area 100</b>							
W101	Coal Receiving/Storage							
W102	Coal Drying/Grinding	-307						600
W103	Shell Gasification		2958		88587		1240	
W105	Sour Water Stripping	-23			732	15	10	
W106	Acid Gas Removal	-126			5612		79	
W107	Sulfur Recovery/TGT	-59	48		411		6	25
W108	Sulfur Polishing							70
W109	Syngas Wet Scrubbing				5460	188	77	
W110	Air Separation	-1621			56890		796	
	Subtotal:	-2136	3006	0	157692	203	2208	695
	<b>Area 200</b>							
W201	F-T Synthesis	-12	3381	119	2092	285	29	5
W202	CO2 Removal	-3180			35250	2414	494	
W203	Dehydration/Compress	-7			1515		27	
W204	Hydrocarbon Recovery	-94		10	3723	144	52	38
W205	Hydrogen Recovery				381		5	
W206	Autothermal Reforming	-2						
	Subtotal:	-3295	3381	130	43361	2843	607	43
	<b>Area 300</b>							
W301	Wax Hydrocracking	-52			224	375	3	91
W302	Distillate Hydrocracking				191	24	3	12
W303	Naphtha Hydrotreating				2867		40	57
W304	Catalytic Reforming		25		761		10	110
W305	C4 Isomerization	-78			69	78	1	2
W306	C5/C6 Isomerization	-5			52		1	3
W307	C3/C4/C5 Alkylation	-63		18	1228	105	17	
W308	Saturated Gas Plant	-7			1204	4	17	11
	Subtotal:	-205	25	18	6596	586	92	285
	<b>Offsites</b>							
W19	Relief and Blowdown							
W20	Tankage							
W21	Intercon. Piping System							
W22	Product Shipping							
W23	Tank Car/Truck Loading							
W24	Coal Refuse/Ash Disposal							
W25	Cat./Chem. Handling							
W31	Steam and Power Gener.	-369			11907		167	312
W32	Raw/Cooling/Pot. Water							
W33	Fire Protection System							
W34	Sewage/Effl. Treatment							0
W35	Instrument/Plant Air							
W36	Purge/Plush Oil System							
W37	Solid Waste Management							
W40	General Site							
W41	Buildings							
W42	Telecommunications							
Other	Miscellaneous	-89						
	Subtotal:	-458	0	0	11907	0	167	312
<b>TOTAL</b>		<b>-6094</b>	<b>6412</b>	<b>148</b>	<b>219555</b>	<b>3632</b>	<b>3074</b>	<b>1335</b>

(-) indicates Production

**Table 2-9**  
**Overall Catalyst and Chemical Requirements**  
**Western (Wyoming) Coal Case**

Catalyst	Plant	Initial Requirement	Annual Consumption
<b>Area 100</b>			
Sulfuric acid, 25 wt%	W105		16,030 lb/hr
Claus (Kaiser S-201)*	W107	3450 cft	690 cft/yr
SCOT catalyst*		1,220 cft	244 cft/yr
2" SS Pall rings*		470 cft	157 cft/yr
MDEA*		94 lbl	9 gal/d
Sulfur polishing (ZnO)	W108	526 cft	111 cft/yr
Caustic, 25 wt%	W109		5,322 lb/hr
<b>Area 200</b>			
FT Ppt. Fe-catalyst	W201	2,302,869 lb	11,514 lb/d
MDEA for CO2 removal	W202	1,211,580 lb	302895 lb/yr
Molecular sieve	W203	155,000 lb	0
Reformer, C14-2	W206	2,766 cu ft	553 cft/yr
<b>Area 300</b>			
UOP LPHC Catalyst	W301	233,900 lb	33,420 lb/yr
NiMo Based Catalyst	W302	34,690 lb	6,940 lb/yr
NiMo Based Catalyst	W303	252,900 lb	50,540 lb/yr
UOP Platform Catalyst	W304	160,600 lb	48,380 lb/yr
3A Molec. Sieve	W305	4120 lb	818 lb/yr
Englehard Isom. Catalyst		11,140 lb	2230 lb/yr
1" Raschig Rings Pack		182 ft3	0 ft3/yr
Carbon Tetrachloride		11,140 lb	1340 lb/yr
Caustic		242 lb	141 lb/yr
KOH		818 lb	5 lb/yr
3A Molec Sieve	W306	8220 lb	1646 lb/yr
Englehard Isom. Catalyst		44,980 lb	9000 lb/yr
1" Raschig Rings Pack		197 ft3	0 ft3/yr
Carbon Tetrachloride		12,330 lb	162 lb/yr
Caustic		270 lb	167 lb/yr
KOH		904 lb	5 lb/yr
H2SO4 (98.5 wt%)	W307	919 ton	37530 ton/yr
Caustic (100% NaOH)		5370 lb	314,600 lb/yr
<b>Offsite</b>			
Alum	W32	19,000 lbs	2,900 lb/d
Polymer		6,000 lbs	1,100 lb/d
98% H <sub>2</sub> SO <sub>4</sub>		9,000 gals	9,900 lb/d
50% NaOH		19,000 gals	24,400 lb/d
Chlorine	W34	2,000 lbs	350 lb/d
Polymer		3,000 lbs	450 lb/d
Pac		6,000 lbs	2,000 lb/d



**Figure 2-1**  
**OVERALL STEAM AND**  
**CONDENSATE DISTRIBUTION**  
**WESTERN (WYOMING) GOAL**  
 Flow Rates Are  
 1000 Lbs/hr

### Section 3

## **Task 2 - Evaluate Baseline and Alternative Economics**

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Preliminary economic analyses were performed on the Baseline Design and the Alternatives cases, using the same set of financial assumptions that was taken directly from the Direct Liquefaction Baseline Study, as requested by DOE. Most of the assumed parameters, however, can be varied in the discounted cash flow (DCF) economic spreadsheet.

Results were compared with each other, and reviewed in the February 2, 1994 Technical Progress Review Meeting. The alternate (ZSM-5) Refining Case has the lowest capital cost and the highest hydrocarbon production per unit of coal feed. The Western Coal Case, on the other hand, has the highest capital and the lowest hydrocarbon product per unit of coal feed. However, the economics expressed in terms of a crude oil equivalent price, favored the Western Coal Case because of its low coal (\$4.5 versus \$24.0 per ton of as received Illinois No. 6 coal) and labor costs.

It is recognized that these preliminary economical analyses did not consider other factors which may have significant impacts on the viability of a F-T coal liquefaction plant. These include : a) the F-T facility's proximity to existing refineries, b) its operating flexibility, and c) the value of its premium upgraded products as blending stocks.

## Section 4

# Task 4 - ASPEN/SP Simulation Model Development

---

Previous quarterly progress reports described the development of ASPEN process simulation models for each of the individual plants in the indirect coal liquefaction complex and their integration into three complete process simulation models for

1. The baseline design case which processes Illinois No. 6 coal at a plant located in southern Illinois
2. An alternate refining case in which the vapor products from the slurry bed Fischer-Tropsch reactors are upgraded in a close-coupled reactor containing ZSM-5 catalyst
3. A Western coal case processing Powder River Basin coal in a plant located in Wyoming.

During this quarter, some of the individual plant models were enhanced, the three complete process simulation models were tuned to the latest utility balances and cost estimates, and the models were tested to verify that they were operable over the required ranges.

As they now stand, the three ASPEN process simulation models essentially are completed and match the current Bechtel designs. However, as a result of the February technical project review meeting, a new Fischer-Tropsch catalyst/wax separation scheme using a Kerr-McGee ROSE unit will be developed, and the models will be revised as appropriate. However, these revisions are not expected to be extensive.

### 4.1 ENHANCEMENTS TO THE 201 FISCHER-TROPSCH SYNTHESIS REACTOR MODEL

The Fortran user block model for Plant 201, the Fischer-Tropsch synthesis plant, is the most sophisticated of all the Fortran user block models. This block model consists of thirteen Fortran subroutines. It models the slurry bed Fischer-Tropsch reactions, predicts the yields, predicts the utilities consumptions and productions for the entire Fischer-Tropsch plant, and sizes the slurry bed reactors.

During this quarter, three revisions were made to this model. These involved extending the model to predict the average wax properties as a function of processing conditions, adding a catalyst activity parameter, and improving the convergence of an internal loop in the reactor sizing routine.

The yields section of the Fischer-Tropsch reactor model was extended to predict the average boiling point and API gravity of the wax. Since this model already predicted the average molecular weight of the wax as a function of reactor temperature (wax

yield), correlations were developed to predict the average boiling point and API gravity of the wax by extrapolating normal paraffin and 1-olefin data to heavier molecular weights. Some minor adjustments to a few additional model parameters were required to compensate for slight shifts in other areas of the plant as a result of using the new wax property predictions.

The Fischer-Tropsch slurry bed reactor sizing model was extended to add a new design parameter, a catalyst activity multiplier. As a result of this addition, the effect of catalyst activity (relative to that of the baseline design) on the size and cost of the slurry bed Fischer-Tropsch reactors now can be studied.

The convergence procedure in the Fischer-Tropsch reactor sizing model was improved to make it more robust. During a sensitivity study which examined the effect of relative catalyst activity on reactor size and cost, a problem was discovered with the original convergence procedure at low relative catalyst activities. Modifications were made to extend the range of catalyst activities which can be studied by improving the stability of this internal convergence procedure.

#### 4.2 REVISIONS TO THE THREE PROCESS SIMULATION MODELS

The three ASPEN process simulation models for the baseline design, alternate refining, and Western coal cases were revised and tuned to match the latest utility balances and cost estimates. Also, some of the summary report files were revised to make them easier to read.

Another revision was made to improve the way the model predicted of the raw water makeup rate. Since most of the water loss occurs by evaporation in the cooling towers, the makeup water rate now is predicted as a function of the total cooling water circulation rate rather than as a function of the coal feed rate.

All three process simulation models were tested over the 5,000 to 50,000 tons/day coal feed rate range to verify that they function correctly over this required range. Some minor adjustments were made to the extend the limits in some ASPEN design specifications and to adjust some maximum unit sizes to obtain adequate behavior over the entire range.

The ASPEN input files for the three process simulation models were cleaned up and additional comments were added to make them easier to follow and use. Additional caveats and warnings were added to the input files to help the user avoid some pitfalls when changing them.

In order to avoid confusing the reader with several versions of preliminary and possibly conflicting results, the ASPEN model results for the baseline design case which were presented in the eighth (July-September '93) Quarterly Report are those for the current plant design. Similarly, the results for the alternate refining case using ZSM-5 catalyst and those for the Western coal case that were presented in the ninth Quarterly Report (October-December '93) are for the current plant designs. Therefore, they are not reprinted here.

Section 5

## **Task 6 - ASPEN/SP Simulation Model Documentation**

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Presentations describing the ASPEN process simulation models and LOTUS spreadsheet economics model were delivered at the February 2, 1994 Technical Progress Meeting.

A draft of the Topical Report for Task IV documenting the ASPEN process simulation models has been prepared. This report documents the models, presents and compares their results with the detailed designs, provides users' instructions for running them on ASPEN/SP, and contains an overview of the LOTUS spreadsheet economics model. A separate restricted addendum has been prepared to document the LOTUS spreadsheet economics model.

This draft report documenting the ASPEN process simulation models will be useful to those individuals converting them from ASPEN/SP to ASPEN PLUS. In addition, this draft report will be used during the model training course which will be given to DOE personnel at PETC after the models have been converted to ASPEN PLUS.

The Topical Report for Task IV and its restricted addendum will be submitted for review by PETC after the final revisions for the improved catalyst/wax separation scheme have been made.

Section 6

## **Project Management & Staffing Report**

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### **6.1 TASK 7 - PROJECT MANAGEMENT**

During this reporting period, cost and schedule control was the primary activity. A technical progress meeting was held at Bechtel San Francisco office on February 2, 1994.

### **6.2 KEY PERSONNEL STAFFING REPORT**

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

<b>Name</b>	<b>Function</b>	<b>% Time Spent<sup>(a)</sup></b>
<b>Bechtel</b>		
Samuel S. Tam	Project Manager	25
Gerald N. Choi	Process Engineer	90
<b>Amoco</b>		
R.D. Kaplan	Subcontract Manager	4
S. S. Kramer	Process Model/Simulation	74

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

Figure 6-1  
Overall Milestone Schedule  
(as of March 13, 1994)

1. TITLE		2. REPORTING PERIOD		3. IDENTIFICATION NUMBER																					
Baseline Design/Economics for Advanced Fischer-Tropsch Technology		2/14/93 to 3/13/94		DE-AC22-81PC0027																					
4. PARTICIPANT NAME AND ADDRESS		5. START DATE		6. COMPLETION DATE																					
Bechtel Corporation 50 Beale Street San Francisco, CA 94105		6/28/91		4/30/94																					
7. ELEMENT CODE	8. REPORTING ELEMENT	9. DURATION												10. PERCENT COMPLETE											
		FY 93						FY 94						Per	Actual										
		M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A
Task 1	Baseline Design	[Gantt bar with markers 1, 2, 3, 4]												100	100										
Task 2	Economic Evaluation	[Gantt bar with marker 5]												100	100										
Task 3	Engineering Design Criteria	[Gantt bar with marker 6]												100	100										
Task 4	Process Flow-sheet Simulation Model	[Gantt bar with marker 7]												74	74										
Task 5	Sensitivity Studies	[Gantt bar with marker 8]												53	53										
Task 6	Documentation and Training	[Gantt bar with marker 9]												10	10										
Task 7	Project Management & Administration	[Gantt bar with marker 10]												82	82										
△	Completion	⑩ Baseline case equipment list transmitted to Cost Estimating																							
①	Second progress meeting																								
②	Baseline case design complete																								
11. SIGNATURE OF PARTICIPANT'S PROJECT MANAGER AND DATE		Samuel S. Tam <i>[Signature]</i> 4/1/94																							

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