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U.S. Department of Energy Pittsburgh Energy Technology Center

Baseline Design/Economics for Advanced Fischer-Tropsch Technology

Contract No. DE-AC22-91 PC90027

Quarterly Report

April – June 1992

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Contents

Section				Page		
1	Intro	duction.		1-1		
2	Sum	Summary				
3	Carb	Carbon Dioxide Removal Tradeoff Study				
	3.1	Introdu	ction	3-1		
	3.2	Chemic	al Solvents	3-2		
		3.2.1	High Concentration MEA	3-2		
		3.2.2	Inhibited Amines	3-3		
		3.2.3	Benfield Hot Potassium Carbonate Process	3-4		
	3.3	Physica	I Solvents	3-4		
		3.3.1	Selexol	3-4		
		3.3.2	Rectisol	3-5		
	3.4	Cryoge	nic - Ryan Holmes Process	3-5		
	3.5	Other I	Processes	3-6		
		3.5.1	Membrane	3-6		
		3.5.2	Membrane Plus PSA/Inhibited Amine	3-6		
		3.5.3	PSA	3-7		
		3.5.4	Exxon Controlled Freeze Zone Process	3-7		
	3.6	Discus	sion and Conclusion	3-7		
4	Pre	liminary	Design for Coal Receiving and Preparation	4- 1		
	4.1	Coal F	Receiving and Storage (Plant 101)	4- 1		
		4.1.1	Design Basis	4- 1		
		4.1.2	Process Description	4-1		
Bacolin	e Shudy	F-T		ii		

Section			P	'age
		4.1.3	Major Equipment List & Utility Summary	4-2
	4.2	Coal D	rying and Grinding (Plant 102)	4-3
		4.2.1	Design Basis	4-3
		4.2.2	Process Description	4-3
		4.2.3	Equipment List and Utility Summary	4-4
5	Preli	iminary	Design for Syngas Production	5-1
	5.1	Shell G	asification - Illinois #6 Coal (Plant 103)	5-1
		5.1.1	Design Basis	5-2
		5.1.2	Process Description	5-2
		5.1.3	Material Balance	5-4
	5.2	Syngas	Wet Scrubbing (Plant 109)	5-4
		5.2.1	Design Basis and Considerations	5-4
		5.2.2	Process Description	5-5
		5.2.3	Material Balance	5-5
	5.3	Syngas	Treating and Cooling (Plant 104)	5-5
		5.3.1	Design Basis and Considerations	5-6
		5.3.2	Technology/Vendor Selection	5-7
		5.3.3	Process Description	5-7
		5.3.4	Materiai Balance	5-8
	5.4	Acid G	as Removal (Plant 106)	5-8
		5.4.1	Design Basis	5-8
		5.4.2	Process Description	5-8

Section			P	age
		5.4.3	Material Balance	5-9
	5.5	Sulfur I	Polishing (Plant 108)	5-9
		5.5.1	Design Basis	5-9
		5.5.2	Process Description	5-10
		5.5 . 3	Material Balance	5-10
6	Task	c 3 - Engi	ineering Design Criteria	6-1
	6.1	Steam	Injection versus External Water Gas Shift	6-1
		6.1.1	Scoping Studies	6-2
		6.1.2	Recommendation for Basis of Design	6-4
	6.2	Alterna	ate Refining Upgrade Process (ZSM-5)	6-5
		6.2.1	Alternative Case Design Basis	6-5
		6.2.2	Prediction of ZSM-5 Conversion and Yield	6-5
		6.2.3	Recommendations	6-7
		5.2.4	Elemental Balance	6-7
7.	Ртој	ject Man	agement	7-1
	7.1	Task 7	- Project Management and Administration	7-1
	7.2	Key Pe	ersonnel Staffing Report	7-1

I.

Tables

Table		Page
3-1	Carbon Dioxide Tradeoff Study Summary of Plant Investment	3-9
3-2	Carbon Dioxide Tradeoff Study Utility Requirements Summary	
3-3	Carbon Dioxide Tradeoff Study Comparison of Operating Cost and Revenues	
4-1	Illinois No. 6 Seam Coal Burning Star Mine Washed Coal Analysis	4-5
4-2	Design Basis and Operating Schedule Plant 101 - Coal Receiving and Storage Illinois No. 6 Coal	4-6
4-3	Major Equipment List Plant 101 - Coal Receiving and Storage Illinois No. 6 Coal	4-7
4-4	Design Basis and Operating Schedule Plant 102 - Coal Drying and Grindfing Illinois No. 6 Coal	4-9
4-5	Material Balance Plant 102 - Coal Drying and Grinding Plant Illinois No. 6 Coal	
4-6	Equipment List Plant 102 - Coal Drying and Grinding Plant Illinois No. 6 Coal	
5-1	Gasifier Feed Coal Analysis Illinois No. 6 Coal	5-11
5-2	Total Plant Material Balance Plant 103 - Shell Gasification Illinois No. 6 Coal	

.

.

Tables (Cont'd)

Table		Page
5-3	Total Plant Material Balance Plant 109 - Syngas Wet Scrubbing Illinois No. 6 Coal	5-13
5-4	COS Hydrolysis and AGR Comparison of One-Stage vs. Two-Stage	5-14
5-5	Total Plant Material Balance Plant 104 - Syngas Treating and Cooling Illinois No. 6 Coal	
5-6	Total Plant Material Balance Plant 106 - Acid Gas Removal Illinois No. 6 Coal	
5-7	Total Plant Material Balance Plant 108 - Sulfur Polishing Illinois No. 6 Coal	5-17
6-1	Effect of Pre-Shift	6-9
6-2	Second Step Yield Prediction	6-11

Tables

Figure		Page
3-1	Process Flow Diagram Showing the Inhibited Amine Process	.3-12
3-2	Process Flow Diagram Showing the Rectisol Process for CO ₂ Removal	.3-13
3-3	Process Flow Diagram Showing the Ryan-Holmes Process for CO ₂ Removal	. 3-14
3-4	Block Flow Diagram Showing the Combined Membrane/PSA Process	.3-15
5-1	Block Flow Diagram for Area 100 - Syngas Production	. 5-18
5-2	Block Flow Diagram Showing A Single Shell Gasification Train (Plant 103)	. 5-19
5-3	Simplified Process Flow Diagram For A Two-Stage COS Hydrolysis/AGR Process Configuration	.5-20
7-1	Overall Milestone Schedule	. 7-2

.

vii

-

.

Figures

Drawing	Page
PFD 191-B-01	Mechanical Flow Diagram Plant 101 - Coal Receiving and Storage Illinois No. 6 Coal
PFD 102-B-01	Process Flow Diagram Plant 102 - Coal Drying and Grinding Illinois No. 6 Coal
PFD 109-B-01	Process Flow Diagram Plant 109 - Syngas Wet Scrubbing Illinois No. 6 Coal5-21
PFD 104-B-01	Process Flow Diagram Plant 104 - Syngas Treating and Cooling Illinois No. 6 Coal
PFD 106-B-01	Process Flow Diagram Plant 106 - Acid Gas Removal Illinois No. 6 Coal5-23
PFD 108-B-01	Process Flow Diagram Plant 108 - Sulfur Polishing Illinois No. 6 Coal5-24

Introduction

Section 1 Introduction

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

The objectives of the study are to:

- Develop a baseline design for indirect liquefaction using advanced F-T technology.
- Prepare the capital and operating costs for the baseline design.
- Develop a process flow sheet simulation (PFS) model.

The baseline design, the economic analysis, and the computer model will be the 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.

This report is Bechtel's third quarterly technical progress report covering the period from March 16, 1992 through June 21, 1992. This is the reporting period covered by the three monthly status reports already published.

This report consists of seven sections:

- Section 1 Introduction
- Section 2 Summary
- Section 3 Carbon Dioxide Removal Tradeoff Study
- Section 4 Preliminary Plant Designs for Coal Preparation
- Section 5 Preliminary Design for Syngas Production
- Section 6 Task 3 Engineering Design Criteria
- Section 7 Project Management

<u>Summary</u>

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Section 2

Summary

This report summarizes the activities completed during the period March 16, 1992 through June 21, 1992 for the tasks scheduled for the period, i.e., Tasks 1, 3, and 7.

In Task 1, Baseline Design and Alternates, the carbon dioxide removal tradeoff study was completed. The inhibited amines process was selected for the baseline design in separating the carbon dioxide from the F-T recycle gas stream.

The material and heat balances, process flow diagrams, and utility balances for these process units were completed during the reporting period:

- Plant 101 Coal Receiving and Storage (Illinois #6 Coal)
- Plant 102 Coal Drying and Grinding (Illinois #6 Coal)
- Plant 103 Shell Gasification (Illinois #6 Coal)
- Plant 104 Syngas Treating and Cooling
- Plant 106 Acid Gas Removal
- Plant 108 Sulfur Polishing
- Plant 109 Syngas Wet Scrubbing

The process units that are in different stages of progress are: sour water stripping, Shell gasification for the Wyoming coal, sulfur recovery, wax/catalyst separation, autothermal reformer, wax hydrocracking, coal preparation for the Wyoming coal, and conventional upgrading.

In Task 3, Engineering Design Criteria, the need of an external water gas shift unit was investigated and the correlation of Mobil's data on ZSM-5 catalyst was developed for the alternate upgrading case. Results from the Viking slurry reactor model and Bechtel's model indicate that the case without pre-shift is a viable case. It should be selected for the baseline design because it is the lowest cost alternative.

A set of design componential conversions and carbon yields was developed for the alternative upgrading case and a typical second stage yield prediction is shown based on these criteria.

Carbon Dioxide Removal Tradeoff Study

Section 3 Carbon Dioxide Removal Tradeoff Study

A series of tradeoff studies on the F-T recycle loop configuration was initiated in the first quarter of 1992. The major objectives of the tradeoff studies are to select the most cost-effective F-T recycle loop configuration for the baseline design through evaluation of various process alternates and to investigate the alternate process units and variables with the greatest impacts on the baseline design.

The process units and process variables studied include:

- Oxygen purity for the Shell gasifiers
- F-T reactor pressure
- Wax yield (F-T reactor temperature)
- Autothermal reforming
- Hydrocarbons (C₃/C₄'s) recovery
- H₂ recovery
- CO₂ removal

With the exception of CO₂ removal, detailed results of the tradeoff study were summarized in the second quarterly (January-March 1992) report. This section summarizes the findings and conclusion on the CO₂ removal unit study.

3.1 INTRODUCTION

In the Fischer-Tropsch (F-T) reaction, a considerable amount of CO₂ is produced (50-65 mol% of FT product) as per reaction 3.1 when the H_2/CO ratio in the feed gas is low.

$$H_2 + 2CO -> -CH_2 + CO_2$$
 (3.1)

The CO_2 must be removed to a low level in order to prevent a buildup of CO_2 in the recycle gas stream which will increase equipment sizes. Excess amounts of CO_2 will also solidify in the cryogenic section of the hydrocarbon recovery plant and plug up the heat exchangers and other equipment.

The optimum place to remove the CO_2 is just before the recycle compressors. This avoids compressing the large amount of CO_2 in the recycle gas. Approximately 20,000 horsepower can be saved in the recycle compressors. The general requirements or preferences for the CO_2 removal unit are: (1) the CO_2 removal system must operate at around 260 psig; (2) the CO_2 stream has to be free of

hydrocarbons and other inert gases so that it can be used in the gasifier coal feed system and vented to the atmosphere without additional treatment; (3) the CO₂ stream is required at high pressure; (4) the CO₂-lean syngas must be free of solvent; and (5) low energy requirement is preferred. The following CO₂ removal processes were investigated:

- Chemical Solvents

 High Concentration MEA
 Inhibited Amines
 Benfield Hot Potassium Carbonate
- Physical Solvents Rectisol Selexol
- Cryogenic Ryan-Holmes
- Others Membrane plus PSA/Amine PSA Only

3.2 CHEMICAL SOLVENT

The major application of the bulk removal of CO_2 from synthesis gas is the production of ammonia and hydrogen from steam-hydrocarbon reforming plants. Because of the pressure level of these plants which is in the 250-350 psig range, the vast majority of these plants use chemical solvents such as amines or alkali carbonates.

3.2.1 High Concentration MEA

In this tradeoff study, a 30-33 wt% MEA solvent with appropriate inhibitors is used to remove CO_2 from the F-T recycle gas. The chemical solvents have an advantage in this application in that they absorb very little of the other components from the recycle gas. There is less than 100 ppmv of hydrocarbons in the CO_2 vent gas.

The CO₂ off gas stream that is not used in the coal drying and transporting sections of the plant can be released to the atmosphere without further treatment. The MEA solvent is a primary amine that is more reactive than the secondary amines such as DEA and tertiary amines such as MDEA. Therefore it can remove CO₂ down to a lower level. However, because it is more reactive it is also more corrosive than the secondary and tertiary amines. Some of the corrosion inhibitors used in the proprietary processes are toxic and there is a concern about disposal of the spent solutions.

The utility requirements, capital and operating costs of this process are shown in Tables 3-1, 3-2, and 3-3, respectively.

3.2.2 Inhibited Amine

There are several proprietary amine solvents such as Gas Spec, UCARSOL, Amine Guard, Textreat, and Flexsorb which contain high concentrations of either MDEA or glycol amines plus proprietary additives. There is not much difference between these processes from a heat requirement standpoint; the major difference is in the types of the corrosion protection schemes. Enquiries were sent to several inhibited amine licensors. Dow's Gas Spec process which uses a 50 wt% MDEA solution plus proprietary additives is selected as a representative process for this tradeoff study.

Some of the main design parameters for the Gas Spec process are:

٠	Amine concentration, wt%	50
٠	Reboiler heat requirement, Btu/mol CO2	52,600
٠	Power requirement, kwh/mol CO ₂	0.21

The flow scheme of a typical inhibited amine process is shown in Figure 3-1.

One of the inhibited amine licensors was asked to investigate an amine process configuration where the rich solution is flashed down to a low pressure so that part of the CO_2 is flashed off. The CO_2 -lean liquid is cooled and returned to the absorber as a semi-lean solution. The rest of the rich solution is thermally regenerated. This configuration has been promoted by BASF for high pressure feed gases. However the licensor found no advantage to this approach for this application. The circulation rate of the semi-lean solution was quite large and not much CO_2 was flashed off in the low pressure letdown drum.

The utility summary, capital and operating costs of this process option are shown in Tables 3-1, 3-2, and 3-3, respectively.

3.2.3 Benfield Hot Potassium Carbonate Process

The Benfield Hot Potassium Carbonate process is a chemical solvent process where the absorption occurs at an elevated temperature of 150 to 200 °F. This process is widely used for carbon dioxide removal in hydrogen plants and has a similar regeneration heat requirement as those for the high concentration amines processes described above. When it is incorporated with some patented options, the external heat requirement can be lowered by 35%. However, UOP, the Benfield licensor, has determined that the Benfield process is not applicable for removing carbon dioxide from the F-T recycle stream. This stream contains 14 mol% carbon monoxide and the CO content is increased to 35 mol% CO after the CO_2 is removed. The high concentration of CO promotes an irreversible reaction with the carbonate solution to form a potassium formate salt. The potassium formate salt has to be purged continuously in order to maintain an acceptable formate level. UOP decided that the loss of the carbonate solution and the disposal of the potassium formate would be unacceptable both economically and environmentally. Thus, no further consideration is given to this process option for CO_2 removal.

SASOL II uses the Benfield process to clean up the effluent gas from fluid bed F-T reactors but the CO concentration in the effluent stream is about 2 vol%. At this CO level, the rate of potassium formate salt formation is slow.

3.3 PHYSICAL SOLVENTS

Physical solvents are good candidates for the bulk removal of certain compounds if they are in high concentrations — which the CO_2 is in this application. However, most of the physical solvents are not very selective as compared to the chemical solvents. Two of the most popular selective physical solvents, Selexol and Rectisol, were investigated.

3.3.1 Selexol

In order to achieve a similar degree of CO_2 removal as that obtained by the 30% MEA process, the Selexol circulation rate has to be 40% higher than that of the MEA. However, its heat requirement is only one-fourth of that for the 30 wt% MEA case. A key consideration in the comparison of the Selexol process with the inhibited amines process is that a considerable amount of heavy hydrocarbons end up in the CO_2 off gas in the Selexol process. The loss of hydrocarbons will reduce the overall product yield.

Baseline Study F-T

UOP, the current licensor of Selexol, estimated that a very high percentage of the C_3 and heavier materials would be absorbed and carried over in the CO_2 stream from the Selexol stripper. Since most of this CO_2 stream is vented to the atmosphere, this stream would need to be incinerated. UOP declined to develop a design for the F-T application because the heavy hydrocarbons cannot be recovered economically from the CO_2 stream.

3.3.2 Rectisol

Bechtel developed the design of a Rectisol plant using ChemCad process simulation software. The objectives were to estimate the utility requirements and to determine the effects of hydrocarbons on the CO_2 removal process. The PTSRK thermodynamic package was used for the methanol system. The process flow diagram of the Rectisol unit is shown in Figure 3-2. The utility requirements are summarized in Table 3-2.

Nitrogen is used in most of solvent strippers for conventional Rectisol plants. For the F-T baseline design, part of the CO₂ stream is being sent to the coal feed system and a non-CO₂ inert gas is not desirable. Thus, nitrogen stripping is replaced by an indirect steam reboiler design for this case. As shown in Table 3-2, the steam requirement is much higher than that for the other CO₂ removal processes.

No further consideration is given to Rectisol for the CO_2 removal because its utility requirement is higher than those of the inhibited amine unit and because of the concern expressed by Lurgi regarding negative effects from the hydrocarbons in the feed stream.

3.4 CRYOGENIC - RYAN-HOLMES

Ryan-Holmes is a low temperature distillation process that uses extractive distillation to recover C_3 and heavier liquids and CO_2 from the F-T recycle gas. The extractive distillation is done with a recycled C_4 + stream. A simplified diagram of this process is shown in Figure 3-3. The compressed and cooled feed gas is dehydrated in a molecular sieve unit. The dried gas is then fed to an extractive distillation tower where a recycled C_4 + stream recovers the C_3 and heavier materials. The overhead from this tower is compressed and fed to a CO_2 recovery column where CO_2 is condensed in the bottom of the recovery column. The C_2 and lighter material from the column overhead is then sent to a demethanizer where additional CO_2 is removed. The demethanizer overhead is heat exchanged with the warm feed to recover the heat and is sent to the autothermal reformer. The demethanizer bottoms joins the recycle additive from the first tower and is fed to

the additive recovery column where C₃ and heavier material is separated from the recycle additive.

One of the advantages of this process is that it eliminates the need for a separate cryogenic hydrocarbon recovery plant. In addition the CO_2 that is produced is available at pressure and does not need to be compressed as much in order to get into the coal feeding system. The major disadvantage is that ethane cannot be recovered from the CO_2 product. Thus, the net hydrocarbon yield from the F-T plant is reduced by about 2.5% as compared to that of the F-T plant with the inhibited amine system.

Another disadvantage of the Ryan-Holmes process is the extremely large electrical power requirement for feed compression and refrigeration loads.

The utility summary, capital and operating costs of this process option are shown in Tables 3-1, 3-2, and 3-3, respectively.

3.5 OTHER PROCESSES

3.5.1 Membrane

Membranes have been proposed recently as the most cost-effective system to remove bulk CO₂ from associated gas for use in Enhanced Oil Recovery (EOR) projects. The main difference between the Fischer-Tropsch reactor effluent and associated gas is the large quantity of hydrogen that is present in the F-T gas. All commercial membranes at present shows poor separation of hydrogen from CO₂. With a four-stage membrane design, the residue gas still contains 14 mol% CO₂ and the CO₂ rich permeate gas contains 19, 19, and 12% of hydrogen, CO, and C₁+ hydrocarbons, respectively.

Membranes are not considered a viable candidate for CO₂ removal in the baseline design because of the excessive loss of syngas in the permeate stream.

3.5.2 Membrane Plus PSA/Inhibited Amine

In this alternative, two additional process units are incorporated with the membrane in order to produce a high purity CO₂ stream and to minimize the losses of syngas and hydrocarbon products. The overall block flow diagram of this scheme is shown in Figure 3-4.

A two-stage PSA unit is used to recover the hydrogen and other hydrocarbons from the permeate stream. Hydrogen is recovered in the first stage. The gas is then recompressed and bulk of the CO_2 is removed in the second stage. The remaining CO_2 in the residue stream is removed in an inhibited amine unit. The function of the membrane unit is bulk removal to reduce the load on the downstream units.

The utility summary, capital and operating costs of this process option are shown in Tables 3-1, 3-2, and 3-3, respectively.

3.5.3 PSA-Only

PSA has been widely used to separate CO_2 from natural gas and other methane-rich gases. However, PSA-only is not feasible for CO_2 removal in the F-T plant because most of the C_2 + is removed from the syngas with the CO_2 . Thus, this process option was not evaluated in detail.

3.5.4 Exxon Controlled Freeze Zone Process

Excon has developed a cryogenic process for separating CO_2 from methane and light hydrocarbon products. Incorporation of this process for F-T CO_2 removal will still require an additional step to remove CO_2 from the C_2 and heavier hydrocarbons. This option was not evaluated in detail because it has not been commercially proven. Its economics should be similar to that of the Ryan-Holmes process.

3.6 DISCUSSION AND CONCLUSION

As discussed above, the physical solvent processes, such as Selexol and Rectisol, are not applicable for removing CO_2 from the F-T recycle gas because of excessive losses of hydrogen, CO, and hydrocarbon components. Moreover, the recovered CO_2 stream has to be treated before it can be used in the coal feeding unit or vented to the atmosphere. For similar reasons, PSA-only and membrane with/without the PSA/amine unit are not attractive options for removing the CO_2 from the F-T recycle gas.

The chemical absorption processes and the Ryan-Holmes process are the most likely candidates for the separation of CO_2 from the F-T recycle gas. The major advantage of the chemical absorption processes is that they only remove CO_2 and there is very little loss of other valuable components. The disadvantage is the high steam requirement for regeneration of the solvent.

The Ryan-Holmes process is also a promising technology for CO_2 removal. As CO_2 is separated from the F-T recycle gas, part of the hydrocarbon is also recovered. This reduces the size and the cost of the downstream hydrocarbon recovery plant. The

main drawback is its high demand of electrical power for the compression and refrigeration of the recycle gas. Another uncertainty is the maximum allowable hydrocarbon content in the CO₂ stream so that it can be vented to the atmosphere without additional treatment, such as incineration. If the CO₂ stream must be incinerated, the Ryan-Holmes process will require an addition of \$10.5 million/year of fuel gas. As shown in Table 3-1, the estimated plant cost for the Ryan-Holmes process is almost twice as high as those of the chemical solvent processes. Utility costs for the Ryan-Holmes and amine systems are considered a stand-off, but the amine systems use low pressure steam rather than power.

The inhibited amine system is selected for the baseline design instead of the Ryan-Holmes process because of its lower capital cost and its ability to utilize abundant, byproduct low pressure steam. It is preferred over the MEA process because it is less corrosive and more reliable.

Table 3-1 Carbon Dioxide Tradeoff Study Summary of Plant Investment (\$ MM)

	Hi Conc. MEA	Inhibited Amine	Ryan Holmes	Membrane /PSA
CO ₂ Removal Unit	91.4	89.2	204.8	10.6
Membrane				43.1
Compression				104.8
PSA Unit				120.0
HC Recovery	21.1	_21.1	3.0	15.9
Total	112.5	110.3	207.8	293.5

Table 3-2 Carbon Dioxide Tradeoff Study Utility Requirements Summary

Desig Feed Feed Feed Feed	Design Basis: Feed Gas Flow rate, MM SCFD Feed Gas Temperature, °F Feed Gas Pressure, psig Feed Gas Composition, mol% :				00 30		
	H ₂ O CO N ₂ C ₂ C ₄ C ₆ +	0.0 14.6 4.8 0.5 0.3 1.4	012 6 1 5 5 2	H_2 CO_2 C_1 C_3 C_5	15.1 60.8 1.3 0.4 0.0	.7 36 37 46 38	
		Hi Conc. MEA	Inhibited Amine	Rectis	ol	Ryan Holmes	Membrane /PSA
Steam, 1000 lb/hr	:						
50 psig saturated		3554	3064	:	806		165
150 psig saturated				5	750		
600 psig, 650°F						210	
Power, Kw (note 1	.)	21,172	18,040) 227	,239	108,000	121,739
Cooling Water, M Btu/hr	1M					210	
Fuel gas for incineration, MM Btu/hr (LHV)						724.4	

Note 1: include power requirement for the HC Recovery Unit

Table 3-3 Carbon Dioxide Tradeoff Study Comparison of Operating Cest and Revenues (\$MM/year)

	Unit Price	Hi Conc. MEA	Inhibited Amine	Rectisol	Ryan- Holmes	Membrane /PSA
Revenues:						
Light Ends	\$1.8/MM Btu	3.0	3.0	2.9	2.4	
C3/C4	\$0.45/gal	35.0	35.0	33.6	33.4	
Gasoline	\$23/Bbl	. 147.0	147.0	141.2	1 43. 7	
Diesel	\$26/Bbl	202 .0	202.0	1 94.3	1 97.2	
Alcohols	\$1.8/MM Btu		2.1	2.0	2.0	
Total		389.5	389.5	373.9	379.8	
Operating Costs:						
Steam	\$/1000 lb					
50 psig saturated	\$1.62	46.4	40.0	75.1		3.4
600 psig, 650°F	\$5.00				8.5	i
Power, Kw (note 1)	5.1 C/Kwh	8.7	7.4	93.4	44.4	48.8
Cooling Water, MM Btu/hr	\$0.67	0.9				<u> </u>
Total		56.0	48.6	168.5	54.9	52.2
Fuel gas for incineration	MM Btu/hr				10.5	5

Note 1: include power requirement for the HC Recovery Unit

Section 3













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Preliminary Design

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for Coal Receiving and Preparation

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Section 4 Preliminary Plant Designs for Coal Preparation

4.1 PLANT 101- COAL RECEIVING AND STORAGE

4.1.1 Design Basis

This plant is intended to receive, store, and reclaim coal from storage, and deliver coal to the Pulverizer Feed Silos in Plant 102. The plant receives washed Illinois No. 6 seam coal from a mine-mouth coal washing plant. The storage and reclaim facilities are designed to ensure a reliable and steady flow of coal to the gasifiers.

Long term coal storage and a conveyor for transporting washed coal to the F-T plant will be provided by the coal mine owner. The analysis of washed coal is shown in Table 4-1. The design bases for the different sections of Plant 101 and their operating schedules are given in Table 4-2.

The design capacity of this plant (20,320 TPD) is based on the requirement of the coal gasification plant (Plant 103). Coal from this plant is ground and dried in Plant 102 before it is sent to the gasifier feeding system.

4.1.2 Process Description (PFD 101-B-01)

The mechanical flow diagram for Plant 101 is shown in PFD 101-B-01. A belt conveyor from a coal washing plant located at the coal mine delivers washed and crushed coal, 2" x 0" in size, to the Receiving Conveyor, 101T-1, which in turn feeds the Stacking Conveyor, 101T-3. The Stacking Conveyor runs along the entire length of the coal storage yard. Coal from the Stacking Conveyor is stacked into two longitudinal piles by a travelling Stacker, 101T-4, which is fitted with a tripper. The boom conveyor of the Stacker has swinging capabilities which enable it to make two piles, one on each side of the Stacking Conveyor. The boom conveyor can also be raised or lowered as required so coal is dropped on the pile from a minimum height. This method of operation minimizes airborne fugitive dust. The coal piles are designed to hold a total of 80,000 tons of coal which is adequate to meet consumption at the gasifiers for approximately four days.

Coal from the longitudinal piles is recovered by a travelling Bridge Reclaimer, 101T-4. The reclaimer, which has a span slightly larger than the width of the piles at the base, travels on rails for the entire length of a pile. It is moved from one pile to the other by a Transfer Car, 101T-8.

The Bridge Reclaimer, which serves both coal piles, reclaims the coal from the entire cross section of a pile using an adjustable scraper. Coal scraped from the pile slides over to a conveyor which is an integral part of the reclaimer. The conveyor

feeds the No. 1 Reclaim Conveyors located along one side of the pile. There are two No. 1 Reclaim Conveyors, 101T-6A and 6B, each serving a pile. Reclaim Conveyor No. 2, 101T-7, collects the coal from the No. 1 Reclaim Conveyor and delivers the coal to either one of the two Silo Feed Conveyors, 101T-14A and B.

An emergency stockpile with its own reclaim system is provided to receive coal and deliver coal to the Silo Feed Conveyors at times when the Stacker and/or Bridge Reclaimer is not available for operation.

A motorized two-way gate located at the delivery end of the Receiving Conveyor, 101T-1, is used to divert the incoming coal to the Emergency Stockpile Conveyor, 101T-10, which makes a conical pile. Coal from the emergency pile is recovered using Bin Activators and Reclaim Feeders, 101T-13, located below the pile in a tunnel. The reclaimed coal is collected from the Emergency Reclaim Conveyor and delivered to one of the two Silo Feed Conveyors.

The Silo Feed Conveyors and the downstream Tripper Conveyors are arranged in two equal capacity trains; normally, one will be operated and the other will serve as a spare.

The Tripper Feed Conveyors, 101T-16A and B, which are fed by the Silo Feed Conveyors, deliver the coal to the Pulverizer Feed Silos in Plant 102. Motorized trippers are used to transfer the coal to the silos. Belt weigh scales are provided at the Silo Feed Conveyors to monitor the coal feed rate to the silos.

To control the fugitive dust, all coal transfer points are fitted with dust extraction systems which consist of dust collectors (baghouses) and exhausters. The collected dust is delivered back to the coal stream. Sumps to collect coal pile runoffs and pumps to deliver the water to a water treatment plant have also been provided.

4.1.3 Major Equipment List & Utility Summary

The major equipment list for Plant 101 is provided in Table 4-3. The list includes all equipment specifications needed to estimate the installed cost of the plant. The total power requirement for this plant is 3,571 KW.

4.2 PLANT 102 - COAL DRYING AND GRINDING

4.2.1 Design Basis

Plant 102 simultaneously dries and grinds the coal for use in the gasifiers. The plant consists of six identical trains. Of these, five are operating trains and the sixth is a spare. Each train has a capacity of 175 short tons per hour (stph) of washed coal. Coal is dried from an initial (as received) total moisture level of 8.6 percent to 2 percent (by weight). The ground or pulverized coal has a size consist of 90 percent passing 88 microns or 170 mesh. The operating schedule of this plant and coal characteristics are shown in Table 4-4.

In the development of the plant designs, two key parameters were investigated: type of inert gas as the drying medium and the final moisture content of gasifier feed coal.

Nitrogen from the air separation plant and carbon dioxide from the F-T reactor loop were the potential candidates as the drying medium in coal drying. Carbon dioxide was considered because it would also be used as carrier gas in the gasifier feed system and would not increase the purge gas flow rate in the F-T reactor loop. Nitrogen was selected for the baseline design for two reasons: (1) there is no combustible impurity in the nitrogen stream; and (2) a negligible amount of nitrogen will be trapped in the ground coal.

The moisture content of the gasifier feed is specified by Shell at 2 wt. % in the Illinois No. 6 coal case. The benefits of keeping the moisture content low are: (a) reduces oxygen consumption in the gasifier and (b) produces less carbon dioxide which is removed in the AGR unit and may dilute the acid gas stream to the Claus plant. The savings in the gasification plant is offset by the increase of fuel gas requirement in the coal drying plant. Shell suggests that the optimized coal moisture content for the Illinois No. 6 coal is about 2 wt. %.

4.2.2 Process Description (PFD 102-B-01)

A process flow diagram for the Plant 102 is illustrated in PFD 102-D-01. There are six trains in the plant. The following description addresses one train.

Coal from the Pulverizer Feed Silo, 102D-1, is fed to the pulverizer by a Weigh Feeder, 102T-1. A closed gas loop consisting of a mixture of air, make-up nitrogen from the air separation plant, and combustion gases is used to dry the coal simultaneously as it is ground in the pulverizer. The gas mixture at 435° F enters the gas inlet connection at the lower portion of the Pulverizer, 102Y-1, and flows upward through the unit. The gases and coal particles entrained by the gases pass through a classifier which is integral with the pulverizer and is located at the upper end of the unit. During this transport, coal particles get dried. At the classifier, coarse particles of coal are separated and dropped back into the grinding zone for further grinding. The dried and ground coal is separated from the gases in a bag filter Dust Collector, 102T-2. The fine coal is collected in an integral hopper in the dust collector. From the hopper, the pulverized coal is delivered to a Pulverized Coal Silo, 102D-2, using a screw conveyor and an air lock.

The Pulverized Coal Silo, 102D-2, is sized to hold 640 tons, equivalent to approximately 4 hours of production from a grinding and drying train. The five silos in the operating trains together can hold 3,200 tons of dried coal which is adequate to supply the eight gasifiers for 4 hours at the design throughput.

The Main Fan, 102K-2, is used to recycle a large bulk of gases from the Dust Collector, 102T-2, outlet. A connection upstream of the Main Fan is provided to vent part of the gases, including moisture evaporated from the coal, to the atmosphere. Downstream of the Main Fan, the recycle gases are mixed with make-up nitrogen and air which provide the carrier for the vented moisture and ensure that the oxygen content in the system is below 7 percent (by volume). It is essential to maintain a low oxygen content in the gases in the circuit to reduce risks of fire and explosion. The mixture of recycle gases, make-up nitrogen, and air are raised to the required mill inlet temperature of 435°F in a Fired Heater, 102F-1, fueled with the purge gas from the F-T reactor loop.

The drying and grinding plant designs were completed in consultation with Losche in Germany. Large capacity (175 stph) pulverizers as offered by Losche are proposed to be used. Losche have several decades of experience in coal and mineral grinding systems. They have supplied coal pulverizers for the Shell gasification plant at Buggenum, Netherlands.

4.2.3 Equipment List and Utility Summary

The major equipment list for Plant 102 is shown in Table 4-6. The list includes all equipment specifications needed to estimate the installed cost of this plant. The total power requirement for this plant is 17,783 KW and the fuel gas required is 230 MM Btu/hr.
Table 4-1

Illinois No. 6 Seam Coal Burning Star Mine Washed Coal Analysis (a)

Item	As Rec'd	Dry Basis	
Higher Heating Value, Btu/lb (measured)	11,193	12,246	
Proximate Analysis, wt %	0.00		
Moisture	8.60	-	
Ash	10.50	11.49	
Volatile Matter	38.60	42.23	
Fixed Carbon	42.30	46.28	
Ultimate Analysis, wt %			
Moisture	8.60	-	
Ash	10.50	11.49	
Carbon	64.90	71.01	
Hydrogen	4.39	4.80	
Nitrogen	1.28	1.40	
Sulfur	2.92	3.19	
Chlorine	0.09	0.10	
Oxygen (by difference)	7.32	8.01	
Ash Mineral Analysis, wt % ash		<u> </u>	
Silica	49.	70	
Alumina	19.	10	
Ferric Oxide	17.50		
Sodium Oxide	0.50		
Potassium Oxide	1.90		
Calcium Oxide	6.	20	
Magnesium Oxide	1.	00	
Titanium Oxide	1.00		
Phosphorous Pentoxide	0.	20	
Sulfur Trioxide	2.	90	

(a) Source: Burning Star Mine

Section 4

Table 4-2 Plant 101 - Coal Receiving and Storage Design Basis and Operating Schedule Illinois No. 6 Coal

(A) Coal Receiving and Storage Section

	Coal consumption for all gasifiers (as received from coal washing plant)	short tons/day	20,320
	Gasification plant - operating schedule:	hrs/day days/week	24 7
	Coal receiving and storage plant - operating schedule:		
		hrs/day da ys/wee k	16 5
	Minimum coal receiving and storage section	short tons/hour	1,778
	Design coal receiving storage capacity	short tons/hour	2,000
(B)	Coal Reclaiming Section		
	Coal reclaiming - operating schedule	hrs/day days/week	24 7
	Minimum reclaiming capacity required Design reclaiming capacity	short tons/hour short/tons hour	1,270 1,500
(C)	Coal Storage Section		
	Coal storage capacity- equivalent days of consumption	days	4
	Coal storage capacity Type of storage	short tons	80,000 Open pile

Item	LD. No.	Title	Qty	Description	Motor HP-Ea	Motor HP- Total
101G-1	А, В	Sump pump	2	Capacity- 200 gpm	15	30
101G-2	A, B, C, D	Runoff pump	4	Capacity- 200 gpm	25	100
101K - 1	Α, Β	Ventilation Fan	2	Capacity 6000 acfin	10	20 [.]
101T - 1		Receiving conveyor	1	Type- Belt conveyor Capacity- 2000 tph Width- 60 in. Length- 200 ft.	75	75
101T-2	A thru E	Motorized gate	5	Type-two way	10/5	30
101 T -3		Stacking conveyor	1	Type- Belt conveyor Capacity- 2000 tph Width- 60 in. Length- 900 ft.	200	200
101T-4		Travelling stacker with tripper	1	Capacity- 2000 tph Belt width- 60 in.	125	125
101 T- 5		Bridge-type reclaimer	1	Capacity- 1500 tph Width- 100 ft.	350	350
101T-6	А, В	Reclaim conveyor No 1	2	Type-Belt conveyor Capacity- 1500 tph Width- 54 in. Length- 900 ft.	100	200
101T - 7		Reclaim conveyor No 2	1	Type-Belt conveyor Capacity- 1500 tph Width- 54 in. Length- 450 ft.	100	100
101T-8		Transfer car	1	Width- 100 ft.	15	15
101T-9		Not used				

Table 4-3 Plant 101 - Coal Receiving and Storage Major Equipment List Illinois No. 6 Coal

Item	I.D. No.	Title	Qty	Description	Motor HP-Ea	Motor HP- Total
101T - 10		Emergency stacking conveyor	1	Type- Belt conveyor Capacity- 2000 tph Width- 60 in. Length- 500 ft.	200	200
101 T - 1 1	A, B, C, B	Bin activator	4	Capacity- 800 tph	25	100
101T - 12	A, B, C, B	Reclaim feeders	4	Capacity- 800 tph	15	60
101T - 13		Emer. reclaim conveyor	1	Type- Belt conveyor Capacity- 1500 tph Width- 54 in. Length- 450 ft.	150	150
101T - 1 4	А, В	Silo feed conveyor	2	Type- Belt conveyor Capacity- 1500 tph Width- 54 in. Length- 500 ft.	250	500
1 01T - 15	Α, Β	Belt scale	2	Type- Belt conveyor Capacity- 1500 tph	0	0
101T - 16	А, В	Tripper conveyor	2	Type- Belt conveyor Capacity- 1500 tph Width- 54 in. Length- 200 ft.	150	300
101T - 17	A, B	Motorized Tripper	2	Motorized tripper Capacity- 1500 tph Width- 54 in.	15	30
101V - 1	А, В	Dust Collector and Fan	3	Air flow- 40,000 acfm	65	195
101V-2	А, В	Sampling System	2	Two stage sampler with surge bin, feeder, crusher, and 2nd stage sampler	25	50
		Total Installed HP				2830

Table 4-3 (continued) Plant 101 - Coal Receiving and Storage Major Equipment List Illinois No. 6 Coal

Baseline Study F-T

Table 4-4 Plant 102 - Coal Drying and Grinding Plant Design Basis and Operating Schedule Illinois No. 6 Coal

Coal consumption for all gasifiers (as received from coal washing plant)	short tons/day	20,320
No. of drying and grinding trains	operating spare	5 1
Minimum capacity required/train Design capacity/train	short tons/hr short tons/hr	169 175
Operating schedule:	hrs/day days/week	24 7

Table 4-5 Plant 102 - Coal Drying and Grinding Plant Material Balance Illinois No. 6 Coal

(Flow rates are for one of five parallel trains)

Stream No.	102.1	102.2	102.3	102.4	102.5	102.6	102.7
Stream Name	Feed	Dried	Vent	Air	Make-up	Recy	Mill
	Coal	Coal	Gases		N ₂	Gases	Outlet
	lbs/hr	lbs/hr	lbs/hr	lbs/hr	lbs/hr	lbs/hr	lbs/hr
Maisture Sma Coal	200 541	200 541					
MUSILIE LIEE COAL	11205	307,741					
Water/Steam	29,125	6,317	24,795			66,199	90 ,994
Oxygen			13,814	13,177	307	36,8 83	50 ,684
Nitrogen			67,274	43,375	47,674	179,612	246,887
Carbon Dioxide			11,117				
Make-Up Nitrogen			47,674				
TOTAL	338,666	315,858	164,674	56,552	47,981	282,694	388,565
Temp Deg F	40	194	214	70	70	214	214
				1	1		

Section 4

Table 4-6 Plant 102 - Coal Drying and Grinding Plant Equipment List Illippis No. 6 Coal

Item I.I No.). Title	Qty	Description	Motor HP-Ea	Motor HP- Total
102D - 1 A Thru 102D - 2 A Thru	F Pulverizer feed silo F Pulverized coal silo	5+1	Capacity- 1400 tons Equivalent cap- 8 hrs. Bulk density - 50 lb/cf Construction - Steel Diameter- 35 feet Cylinder height- 60 feet Bottom cone-25 feet Bottom clearance- 25 feet Top Elevation 110 feet Capacity- 640 tons Equivalent cap- 4 hrs. Bulk density - 35 lb/cf Construction - Concrete Diameter- 25 feet Cylinder height- 80 feet Rottom cape Elat bottom		
102F - 1 A Thru	F Fired heater	5+1	Bottom clearance- 15 feet Top elevation 95 feet Fuel- Gas, 300 Btu/scft Heat release- 50 MMBtu/hr		
102K - 1 A Thru	F Burner air blower	5+1	Gas flow-8000 acfm	150	900
102K - 2 A Thru	F Main fan	5+1	Gas flow-160,000 acfm , Temp. 215 deg. F	2500	15,000
102K - 3 A Thru	F Vent fan	5+1	Gas flow-55,000 acfm , Temp. 215	150	900
102K - 4 A Thru	F Make-up nitrogen fan	5+1	Gas flow- 25,000 acfm , Temp. 70 deg. F	450	2,700

Table 4-6 (continued) Plant 102 - Coal Drying and Grinding Plant Equipment List Illinois No. 6 Coal

	ltem I.D. No.	Title	Qty	Description	Motor HP-Ea	Motor HP- Total
1 02T - 1	A Thru F	Weigh feeder	5+1	Capacity- 200 tph	5	30
102T - 2	A Thru F	Dust collector	5+1	Gas flow- 210,000 scfm Filter Area- 70,000 sq. ft.	10	60
102T - 3		Mill area crane	1	Capacity- 10 tons	25	25
102T - 4	A Th ru F	Vent dust collector	5+1	Gas flow– 250 scfm Filt er Area– 70 sq. ft.	3	18
102Y - 1	A Thru F	Pulverizer	5+1	Capacity- 175 tph Feed Size- 2 in. x 0 Product- 90 % below 88 microns Feed moisture- 8.6% Product moisture- 2% Accessories- Feed screw, Classifier	2,500	15,000

Section 4









Preliminary Design for Syngas Production

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Section 5 Preliminary Design for Syngas Production

The process units within the syngas production plant are grouped in Area 100. They are:

Plant <u>Number</u>	Plant Description
101	Coal Receiving and Storage
102	Coal Drying and Grinding
103	Shell Coal Gasification
104	COS/HCN Hydrolysis
105	Sour Water Stripping
106	Acid Gas Removal (AGR)
107	Sulfur Plant (Claus/TGT)
108	Sulfur Polishing
109	Syngas Wet Scrubbing
110	Air Separation

The block flow diagram for these process plants is shown in Figure 5-1. The overall material balance is found in Tables 5-2, 5-3, 5-5, 5-6 and 5-7. Process designs for Plants 101, 102, 103, 104, 106, 108, and 109 have been completed. Detailed descriptions of Plants 101 and 102 were provided earlier in Section 4 of this report. Details for the remaining plants are included in this section.

5.1 PLANT 103 - SHELL GASIFICATION - ILLINOIS NO. 6 COAL

Plant 103 is designed to gasify washed, dried Illinois No. 6 coal for the production of a medium Btu syngas. The process design, material and heat balance, utility requirements, and installed plant cost were prepared by Shell Oil Company. Bechtel developed the design basis and assisted in the integration of the Shell gasification plant with the rest of the F-T plant. Below is a summary of the non-proprietary description of Plant 103 for this F-T baseline study.

5.1.1 Design Basis

An integral number of single Shell gasifiers of maximum size is selected for the baseline design. Based on the most recent experience with their gasifier, Shell has determined that the maximum size single gasifier will handle an equivalent of 2,540 short tons per day of Illinois No. 6 coal on an "as received" basis. The design basis for Plant 103 is:

<u>Category</u>

Design Basis

Number of operating gasifiers Coal feed rate to each gasifier Moisture content in gasifier feed coal Feed coal size Inert gas for coal feeding Oxygen purity Slag disposal

8 2,540 stpd (as received basis) 2 wt. % 90% below 88 microns carbon dioxide 99.5 mol % Return to mine for on-site disposal

Carbon dioxide is used as carrier gas in order to reduce inerts buildup in the F-T loop. Analysis and composition of the dried feed coal to the gasifier are shown in Table 5-1.

The sensible heat from the syngas is recovered for the production of 900 psig, 1000°F superheated steam. Most of this steam is used to drive the air compressors in the Air Separation Plant (Plant 110).

5.1.2 Process Description

There are eight parallel operating gasifier trains. Figure 5-2 is the block flow diagram showing one Shell gasification train which consists of the following sections: milled coal pressurization and feeding, gasification and gas quench, high temperature gas cooling and flyslag removal, slag handling, flyslag handling, and solid waste handling.

Milled Coal Pressurization and Feeding

The milled and dried coal from Plant 102 is pneumatically transported to the coal pressurization and feeding system. This system consists of a receiving vessel, two lock hoppers, and a feed hopper. The receiving vessel separates the coal from its carbon dioxide transport medium and then transfers the coal to one of the two lock

carbon dioxide transport medium and then transfers the coal to one of the two lock hoppers. These two lock hoppers are operated on a time cycle such that one is filled and pressurized while the other is emptied and depressurized. Once a lock hopper has been charged with coal from the receiving vessel, it is then pressurized with carbon dioxide and its contents are discharged into the feed hopper. Pressurized coal is continuously withdrawn from the feed hopper and pneumatically conveyed with carbon dioxide to the gasifier's coal burners.

Gasification and Gas Quench

Pressurized coal, oxygen and steam enter the gasifier through opposed burners. The gasifier consists of an outer pressure vessel and an inner, water-cooled membrane wall. The gasifier wall temperature is controlled by circulating water through the membrane wall to generate saturated steam for subsequent superheating in the syngas cooler. The membrane wall encloses the gasification zone from which two outlets are provided: one opening at the bottom of the gasifier is used for the removal of slag; the other opening allows hot raw gas to exit from the top of the gasifier.

Most of the mineral content of the feed coal leaves the gasification zone in the form of molten slag. The high gasifier temperature (up to 3000°F) ensures that the molten slag flows freely down the membrane wall into a water-filled compartment at the bottom of the gasifier.

As the molten slag contacts the water bath, the slag solidifies into dense, glassy granules. These slag granules fall into a collecting vessel located beneath the slag bath and are transferred to a pair of lock hoppers which operate on a timed cycle to receive the slag. After a lock hopper is filled, the slag is washed with clean makeup water to remove entrained gas and any surface impurities. After washing, the lock hopper is depressurized and the slag is fed to a dewatering bin. This bin is equipped with an inclined screw to lift the settled solids off the bottom of the vessel and deposit them on a conveyor belt for delivery to off-site storage and disposal facilities.

The hot raw product gas leaving the gasification zone is guenched with cooled, recycled product gas to convert any entrained molten slag to a hardened solid material, called flyslag, prior to entering the syngas cooler.

High Temperature Gas Cooling and Flyslag Removal

The syngas cooler recovers high-level heat from the quenched raw gas by generating superheated high-pressure steam (900 psig, 1000°F). The syngas cooler includes superheat, evaporative, and economizer sections.

The bulk of the flyslag contained in the raw gas leaving the syngas cooler is removed from the gas using ceramic filters. The recovered flyslag is then recycled back to the gasifier via the coal feeding system or leaves the process as a coproduct similar to the slag. If not recycled, the flyslag leaving the process is pneumatically conveyed to one of two flyslag lock hoppers. After a lock hopper is filled, the flyslag is purged with high pressure nitrogen to remove any entrained raw gas. After purging, the lock hopper is depressurized and the flyslag is pneumatically conveyed to an ash silo for intermediate storage. All vent gases from the flyslag lock hoppers and the storage silo are filtered of particulates during discharge. Then, they are flared at the incinerator located in the Claus plant tail gas treatment section.

5.1.3 Material Balance

The overall detailed material balance for Section 103 is shown in Table 5-2.

5.2 PLANT 109 SYNGAS WET SCRUBBING

The function of this plant is to remove the trace amount of fine particulates in the syngas and to humidify the syngas for COS hydrolysis.

5.2.1 Design Basis and Considerations

After the removal of coarser flyslag particulates from the Shell high temperature cooling/solid removal section of the Coal Gasification Plant (Plant 103), the raw gas is sent to a Venturi type wet scrubber to capture the remaining finer particulates. The water from the ammonia stripper bottoms in Plant 104 (Syngas Treating and Cooling) is used as the source of water for the Venturi atomizers.

The COS in the scrubbed gas will be subsequently hydrolyzed to begin a series of sulfur removal steps. Both lower reaction temperature and higher steam-to-dry-gasratio favour the equilibrium COS hydrolysis reaction:

$$COS + H_2O = CO_2 + H_2S$$

An additional design consideration for Plant 109 is to moisturize the scrubbed gas for the subsequent COS hydrolysis step. The COS hydrolysis reaction temperature is normally set at 30 to 50°F above the reactor feed dew point temperature. Thus, the circulation of the return water in the wet scrubber will be such that the raw gas will be fully saturated to its adiabatic dew point of 255° F. The scrubbed gas is then heated up about 45°F above its dew point to the desired COS hydrolysis reaction temperature of 300°F. The number of parallel trains for Plant 109 is set at eight based on considerations of consistency with the number of upstream gasification trains and downstream number of hydrolyzer reactor trains to simplify interconnecting piping and enhance controllability.

5.2.2 Process Description (PFD 109-B-01)

The process flow diagram for Plant 109 is shown in Drawing PFD 109-B-01. The raw gas at 460°F from the Shell high temperature cooling/bag filter section of the Coal Gasification Plant is cooled by the cold scrubbed gas at Raw Gas/Scrubbed Gas Heat Exchanger 109E-1 before it is sent to a Venturi-type Wet Scrubber, 109V-1. The Venturi atomizing water is drawn from the bottom of the Separator, 109C-1, at a flow rate of 125 gpm, enough to ensure complete water saturation for the raw gas.

The gas/water mixture enters near the bottom of the Separator to disengage the free water. The water from the ammonia stripper bottoms in Plant 104 is introduced near the top of the Separator in order to provide countercurrent flow, and an added washing effect. Most of the combined water stream leaving the bottom of the Separator is recirculated back to the Scrubber and used in the Venturi atomizers. The water blowdown from the Separator is sent to the Sour Water Stripper (Plant 105).

The scrubbed gas leaves the top of the Separator at 255°F. The steam to dry gas ratio (mole/mole) at this point is increased from 0.0317 to approximately 0.09. The scrubbed gas is heated to 300°F, which is 45°F above its water dew point in the feed/effluent cross exchanger, 109E-1. This heated scrubbed gas is sent to the COS hydrolysis reactor in Plant 104.

5.2.3 Material Balance

The overall material balance for the Syngas Wet Scrubbing Plant 109 is shown in Table 5-3.

5.3 PLANT 104 SYNGAS TREATING AND COOLING

The objectives of this plant are to convert the COS in the syngas to H_2S and to cool the syngas before it is fed to the AGR plant (Plant 106). Any HCN in the syngas is also hydrolyzed to ammonia.

5.3.1 Design Basis and Considerations

The particulate-free syngas is sent to this plant as the first step toward sulfur removal. Sulfur is a poison to the F-T catalysts and must be reduced to less than 1 PPMV. The COS has to be converted to H_2S via the hydrolysis reaction before it can be absorbed by the solvent in the downstream Acid Gas Removal (AGR) unit (Plant 106). Otherwise, COS will cause solvent degradation problems via irreversible chemical reactions with the solvent or will slip through the AGR unit.

The COS concentration of the syngas is reduced catalytically to less than 1 PPMV by reacting with steam in the presence of hydrolysis catalyst. Equal molar amounts of H₂S and CO₂ are produced.

In the hydrolysis reactor, the HCN in the syngas can be either hydrolyzed to NH₃ or hydrogenated to methylamine (CH₃NH₂) depending upon conditions and the characteristics of the hydrolysis catalyst. The reaction pathway to NH₃ is assumed for the process design based on information provided by Shell Oil Company. Because of the presence of HCN in the syngas stream only HCN-tolerant COS hydrolysis catalysts are considered.

There are eight parallel trains in Plant 104. The number of parallel trains used is determined by these factors: maximum allowable vessel size due to transportation considerations, allowable gas superficial velocity, and design gas residence time.

Since COS hydrolysis is a reversible reaction, the cost/benefit of a single-stage versus a two-stage COS hydrolysis process configuration was analyzed. The process configuration of a two-stage COS hydrolysis process is shown in Figure 5-3.

A first-stage COS hydrolysis step is followed by partial removal of H₂S in the first AGR absorber. A reduction of H₂S content in the feed stream to the second stage COS hydrolysis will have a favorable effect on the COS hydrolysis equilibrium conversion because H₂S is one of the products in the COS hydrolysis reaction. This results in savings on the usage of total COS hydrolysis catalyst over the single-stage design. Moreover, since all the HCN is converted to ammonia in the first-stage, less expensive COS hydrolysis catalyst can be used for the second stage.

The drawbacks of the two-stage design are higher equipment and operating costs and higher pressure drop in the syngas production plant. The resulting lower system pressure will increase the equipment sizes within the FT synthesis plant and the accompanying F-T recycle loop.

Table 5-4 lists the differential costs of the one- and two-stage COS hydrolysis designs. As shown, the investment for the two-stage design is \$718,000 higher than that for the one-stage design. The annual operating cost of the two-stage design is also higher because the savings on the COS hydrolysis catalyst is more than offset by the increased steam and power cost. In the two-stage design, additional steam is needed to reheat the syngas after the first-stage AGR absorber. Power consumption is also increased due to the higher recirculation rate in the AGR unit.

An increase of 25 psi in pressure drop in the syngas gas system for the two-stage design will result in a decrease in the F-T reaction and recycle loop pressures. At an F-T synthesis loop pressure of 315 psia, for example, this represents an increase of 8% in the equipment size. A one-stage COS hydrolysis design is incorporated in the baseline design because both capital and operating costs are lower. The only real argument for the two-stage design is to increase operating flexibility.

Eight operating hydrolysis trains will be installed for the baseline case with Illinois #6 coal. Total initial catalyst loading is estimated to be 43,920 cubic feet corresponding to a space velocity of 1,258 SCF/Hr/SF. The expected average life of catalyst is about 3 years.

5.3.2 Technology/Vendor Selection

There are two major catalyst vendors who can provide the COS hydrolysis catalysts: United Catalysts Inc. of Louisville, KY and Haldor Topsoe, Inc. of Houston, TX.

Catalyst C53-2-01 from United Catalysts Inc or CKA from Haldor Topsoe, Inc. are both considered applicable. Both are HCN tolerant. Catalyst C53-2-01 is used for the baseline design.

5.3.3 Process Description (PFD 104-8-01)

The process flow diagram of the COS hydrolysis plant (Plant 104) is shown in Drawing PFD 104-B-01. The scrubbed gas at 300°F is passed through the Hydrolyzer Reactor, 104C-1, where the COS content is reduced to 1.0 PPMV. The hydrolyzer effluent at approximately 300°F is subsequently cooled down to 100°F through three heat exchangers: 104E-1 with the sweet syngas exiting AGR, 104E-2 with air, and 104E-3 with cooling tower water. The cooled reactor effluent is sent to Separator, 104C-2. The condensed aqueous phase is sent to the NH₃ Stripper, 104C-3 where process water is recovered for use in the Syngas Wet Scrubbing (Plant 109). The vapor phase is sent to the AGR unit (Plant 106) for H₂S removal. The stripped gas from the NH₃ Stripper is sent to the Sulfur Plant (Plant 107) for disposal.

5.3.4 Material Balance

The overall material balance of Syngas Cooling and Treating (Plant 104) is shown in Table 5-5.

5.4 PLANT 106 ACID GAS REMOVAL

The purpose of this plant is to selectively remove H_2S from the syngas down to 4 PPMV while minimizing CO_2 removal.

5.4.1 Design Basis

The minimum H_2S concentration in the acid gas stream to the sulfur plant is 33 vol%. Due to the relatively high CO_2 content in the syngas, a selective H_2S removal process is required. Reboil heat duty should be minimized.

The "pure gas" (or sweet gas) will have a H_2S concentration of 4 ppm by volume on a dry basis. The exit temperature of the sweet gas is 110°F. The resulting H_2S content in the acid gas is estimated to be 42 vol% (dry basis) by UOP, adequate as feed to the sulfur plant (Plant 107).

There are four parallel trains for Plant 106. The number of AGR trains is determined so that one AGR train can handle the syngas output from two gasifiers. The size of the AGR absorber must meet the maximum vessel size criterion (less than 17 feet outside diameter for the Illinois site). The size of Amine Absorber 106E-1 is estimated to be 14'-3" ID and that for Amine Stripper 106E-2 to be 9'-9" ID.

The UOP Amine Guard FS process is selected since it meets all the design requirements at reasonable cost.

5.4.2 Process Description (PFD 106-B-01)

The process flow diagram for the AGR plant (Plant 106) is shown in Drawing PFD 106-B-01. The UOP Amine Guard SF unit is configured similarly to other typical amine units except that a proprietary amine solvent is to be used for acid gas removal. The syngas feed is sent to a location beneath the bottom tray in Absorber 106C-1 where H₂S and, to some extent, CO₂ are picked up by the countercurrent Amine Guard absorbent. The sweet gas leaves at the top of the absorber with a maximum H₂S concentration of 4 PPMV. The trace amount of COS in the feed gas is not picked up by the Amine Guard absorbent, and will stay in the sweet gas. Thus,

the combined sulfur (H_2S plus COS) content in the sweet gas is about 5 PPMV. This will be removed in the sulfur polisher (Plant 108).

The H₂S-laden rich amine solution is heated up in the Lean/Rich Amine Solution Heat Exchanger 106E-2 by the regenerated lean amine from the Amine Stripper, 106C-2. The H₂S is stripped indirectly with 50-psig saturated steam in the Amine Reboiler, 106E-3. The regenerated lean amine solution is cooled to its final temperature of 108°F in a trim water cooler, 106E-1 before it returns to the Absorber. A slip stream of the lean amine solution is sent to the Amine Filters, 106Y-1/2, in order to purge any solids formed due to solvent degradation.

The acid gas, leaving at top of the Amine Stripper, 106C-2, passes through the Acid Gas Condenser, 106E-4 and Acid Gas Knock-out Drum, 106C-4. The liquid from 106C-4 is refluxed back to the stripper and the vapor is delivered to the Sulfur Plant (Plant 107) for sulfur recovery.

5.4.3 Material Balance

The overall material balance of the Acid Gas Removal unit (Plant 106) is shown in Table 5-6.

5.5 PLANT 108 SULFUR POLISHING

The purpose of the sulfur polishing plant is to remove the trace amount of sulfur compounds from the syngas before it enters the F-T reactors. The F-T catalyst can be poisoned by sulfur compounds, such as H_2S , COS and CS₂.

5.5.1 Design Basis

The sweet gas from the AGR unit contains approximately 5 PPMV of total sulfur (COS plus H_2S). This trace amount of sulfur is finally removed in fixed bed reactors loaded with zinc oxide (ZnO) catalyst. The ZnO reacts chemically with H_2S to form solid zinc sulfide (ZnS). The ZnO catalyst will be permanently consumed and eventually replaced.

In order to provide a continuous H_2S pick-up even when H_2S breakthrough occurs, a reactor configuration of two beds in series is used in the process design. The necessary piping is provided so that these two beds can be switched without any interruption of the normal operation. When H_2S breakthrough occurs in the lead bed it is taken off-line for catalyst change-over and the lag bed is in service alone. After changeout, the lead bed, with freshly loaded catalyst, is put back in line as the lag bed. The two-bed-in-series operation continues until the other bed has breakthrough and is taken off-line for a catalyst change-over. The operating cycle repeats. Desired cycle length is 2 years before replacement of one bed.

The G-72D ZnO catalyst from United Catalysts has been selected because it can hydrolyze the light sulfur compounds, such as CS₂, to H₂S at 650 to 700°F and subsequently absorb the H₂S in the same reactor. Therefore, a mixed bed using a CoMo and ZnO is unnecessary.

For the reactor configuration of two beds in series, the ZnO usage rate is typically set at approximately 85 mol COS/100 mcl ZnO, or at an equivalent 21 pounds of sulfur loading per cubic foot of catalyst volume. The sizing of the ZnO fixed-bed reactors is principally dictated by the reactor pressure drop considerations. The ZnO catalyst bed will normally be operated at 650°F and a space velocity of 1,500 SCF/Hr/CF.

5.5.2 Process Description (PFD 108-B-01)

The process flow diagram of the sulfur polishing unit (Plant 108) is shown in Drawing PFD 108-B-01. The feed gas from the AGR unit will be heated to the reaction temperature of 650°F in successive heat exchangers and a fired heater. Sweet gas at 108°F from the AGR unit is preheated to 258°F by cross exchanging with the bottom stream of the COS hydrolyzer. It is then heated to 360°F and 580°F in the F-T Effluent/Feed Exchanger, 108E-2, and the ZnO Effluent/Feed Exchanger, 108E-1, respectively.

The syngas is heated to its reaction temperature of 650°F in the Fired Heater, 108F-1. The total absorbed duty per train for this normal operation is estimated to be 7.5 MMBtu/hr. The total design absorbed duty for each fired heater is 41.9 MMBtu/hr to account for the fact that, during the initial start-up, both heat exchanges with F-T reactor vapor effluent (108E-2) and the ZnO reactor effluent (108E-1) will not be available.

Eight parallel trains, each with two reactor vessels, 14'-0" ID by 10'-0" tangent to tangent, will be installed. The pressure drop across both vessels is estimated to be 10 psi. The catalyst inventory for both beds is about 4,128 cubic feet per train. The expected replacement rate is calculated to be 100% change-over every four (4) years.

5.5.3 Material Balance

The overall material balance for the Sulfur Polishing unit (Plant 108) is shown in Table 5-7.

Table 5-1

Gasifier Feed Coal Analysis (Illinois No. 6 Coal)

	Gasifier Feed	
Item	Coal	Dry
Higher Heating Value, Btu/lb (measured)	11,193	12,246
Proximate Analysis, wt %		
Moisture	2.00	-
Ash	11.26	11.49
Volatile Matter	41.39	42.23
Fixed Carbon	45.35	46.28
Ultimate Analysis, wt %		
Moisture	2.00	-
Ash	11.26	11.49
Carbon	69.59	71.01
Hydrogen	4.70	4.80
Nitrogen	1.37	1.40
Sulfur	3.13	3.19
Chlorine	0.10	0.10
Oxygen (by difference)	7.85	8.01

Table 5-2 Total Plant Material Balance Plant 103 - Shell Gasification (Illinois No. 6 Coal)

Stream No.	103.1 Feed Coal	193.2 Carbon Dioxide	103.3 Oxygen Feed	103.4 Syngas to Scrubbing	103.5 Slag
Phase Flow Rate 1h/hr	Solid	Vap	Vap	Vap	Liq/Solid
H2				67.187	
N2			6,145	27,054	
O2			1,340,997		
H ₂ S				45,587	
ω				2,584,836	
CO2		307,030	1	242,395	
H2O (or Moisture)	31,598			69,416	
COS				7,245	
				424	
				1,2.3± 813	
CHA		ſ	ĺ	367	
Coal MAF	1_370.107				
Ash	177,826			73	177,753
C C				18	6,281 305
Sulfur NaOH				1	2,694
NaCl H2SO4					
Total Lb/hr	1,579,531	307,030	1,347,142	3,046,670	187,033

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Section 5

Table 5-3 Total Plant Material Balance Plant 109 - Syngas Wet Scrubbing (Illinois No. 6 Coal)

Stream No.	109.1	109.2	109.3	109.4	109.5
	Syngas to	Syngas to	Make-up	B/D to	Make-up
	Scrubbing	COS	Water to	SWS	NaOH to
		Hydrolysis	Scrubbing		Scrubbing
Phase	Vap	Vap	Liq	Vap	Liq
Flow Rate, lbmol/hr					
H2	33330.45	33330.09		0.36	
N2	965.74	965.74			
O2					
H2S	1337.81	1319.67		18.14	
Ö	92281.29	92281.28		0.01	
CO2	5507.77	5494.65		13.12	
H2O (er Moisture)	3853.18	12010.30	11621.33	3704.88	206.28
COS	120.62	120.62			
NH3	24.87	25.68	1.57	0.76	
HCI	34.39				
HCN	30.07	29.01		1.06	
CH4	22.88	22.88			
Coal MAF					
Ash	(73 lb/hr)			(73 lb/hr)	
С	(18 lb/hr)			(18 lb/hr)	
) a					
Sulfur	(1 lb/hr)			(1 lb/hr)	
NaOH	[1	34.39	30.76	30.76
NaCl				34.39	
H2SO4					
Total	137509.07	145599.92	11657.29	3803.48	237.04
GPM @T,P			422	152	8
Mol. wt.	22.16	21.92			1
MMSFCFD	1252.43	1326.12			

() = Solids

Baseline Study F-T

Section 5

Table 5-4 COS Hydrolysis and AGR Comparison of One-Stage vs. Two-Stage (Basis: One Gasifiers)

	One-Stage	Two-Stage
Total Installed Cost, \$	-	-
COS Hydrolysis System	Base	1,291,000
AGR	Base	200,000
COS Cat. Initial Charge	2,559,000	1,786,000
Differential	Base	718,000
Operating Cost, \$/yr		
Catalyst (3 yr. life)	853,000	595,000
Steam (\$7/Mlb)	Base	294,000
Power (5.1¢/KWH)	Base	26,000
Differential (Incl. steam cost)) Base	62,000
Pressure Drop, psi	Base	25.0

Table 5-5 Total Plant Material Balance Plant 104 - Syngas Treating and Cooling (Illinois No. 6 Coal)

Stream No.	104.1	104.2	104.3	104.4	104.5
	Syngas to	NH3 Gas	Syngas to	Make-up	Make-up
	COS		AGR	Water to	NaOH to
	Hydrolysis			Scrubbing	NH3
					Scrubbing
Phase	Vap	Vap	Vap	Liq	Liq
Flow Rate, Ibmol/hr					
H2	33330.09	1.31	33328.78		
N2	965.74		965.74		
O2					
H ₂ S	1319.67	13.87	1426.28		
a a construction of the co	92281.28	2.79	92307.16		
CO2	5494.65	48.77	5566.36		
H2O (or Moisture)	12010.30	87.77	381.98	11621.33	229.93
cos	120.62		0.14		
NH3	25.68	52.53	0.25	1.57	
НСІ					
HCN	29.01	0.34			
CH4	22.88		22.88		
Coal MAF					
Ash					
C C					
a					
Sulfur]	
NaOH				34.39	34.39
NaCl					
H2SO4		ļ			
Tatal	145500 60	207.20	122000 57	11/57.30	264.20
CDMATD	140079.92	207.38	10.5444661	11057.29	204.32
Grmei,P	1 21 02	24.00		422	9
MOL WL	21.92	24.99	22.24		ļ
MMSFCFD	1326.12	1.88	1220.47	l	

Baseline Study F-T

Stream No.	106.1	106.2	106.3
	Syngas to AGR	Sweet Gas to	Acid Gas to
	Absorber	Sulfur Polishing	Sulfur Recovery
Phase	Vap	Vap	Vap
Flow Rate, lbmol/hr	-	_	_
H2	33328.78	33294.77	34.01
N2	965.74	965.08	0.66
O2		•	
H2S	1426.28	0.51	1425.77
CO I	92307.16	92245.25	61.91
CO2	5566.36	3816.68	1749.68
H2O (or Moisture)	381.98	472.75(1)	146.58
COS	0.14	0.14	
NH3	0.25		0.25
HC1			
HCN			
CH4	22.88	22.88	
Coal MAF			
Ash			
C			
a			
Sulfur			
NaOH			
NaCl			
H2SO4			
Total	133999.57	130818.06	· 3418.86
GPM @T,P			
Mol. wt.	22.24	21.82	38.04
MMSFCFD	1220.47	1191.49	31.14

Table 5-6 Total Plant Material Balance Plant 106 - Acid Gas Removal (Illinois No. 6 Coal)

(1) Includes moisture pick-up from the amine solution.

Plant 108 - Sulfur Polisning (Illinois No. 6 Coal)				
Stream No.	108.1 Syngas to ZnO Bed	108.2 Syngas to F-T Reactors		
Phase Flow Rate, lbmol/hr	Vap	Vap		
H2	33294 77	33294.77		
N2	965.08	965.08		
O2				
H2S	0.51			
ω	92245.25	92245.25		
CO2	3816.68	3816.68		
H2O (or Moisture)	472.75	472.75		
cos	0.14			
NH3				
HCI				
HCN				
CH4	22.88	22.88		
Coal MAF				
Ash				
C				
a				
Sulfur				
NaOH				
NaCl				
H2SO4				
Total	130818.05	130817.41		
GPM @T,P				
Mol. wt.	21.82	21.82		
MMSFCFD	1191.49	1191.48		

Table 5-7 Total Plant Material Balance Plant 108 - Sulfur Polishing (Illinois No. 6 Coal)



Baseline Study F-T
















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Engineering Design Criteria

Section 6 Task 3 - Engineering Design Criteria

6.1 STEAM INJECTION VERSUS EXTERNAL GAS SHIFT

One of the distinct merits envisioned for the slurry F-T reactor using iron based catalyst is that it can handle the low H_2/CO ratio synthesis gas produced in a coal gasifier. Ideally, with complete water gas shift (WGS), the synthesis reaction becomes:

 $H_2 + 2CO \leftrightarrow -CH_2 - + CO_2$

The stoichiometric H_2/CO ratio in this equation is 0.50. In practice, equilibrium and rate limitations result in some water production and the stoichiometric ratio is more like 0.67.

The Shell gasifier produces a particularly low H_2/CO ratio, on the order of 0.45 and, when CO_2 is used as carrier gas (as in the baseline design), the synthesis gas has a H_2/CO ratio of 0.36. Even with the recycle of gas from an autothermal reformer in the synthesis loop, the H_2/CO ratio remains well below stoichiometric. This can be compensated for by the addition of water vapor and, in the proposed baseline design, 3.72 moles of water vapor are added per 100 moles of fresh feed plus recycle. This water reacts with excess CO and the overall H_2/CO consumption ratio becomes close to that in the feed. An additional result is that the hydrogen concentration in the recycle gas rises to 40%, sufficient for hydrogen recovery in a PSA unit. Basically, what is being done is to carry out additional water gas shift in the F-T reactor, consuming water and producing additional CO₂.

While this would appear to be the most attractive solution from a cost standpoint, objections have been raised that:

- 1. The low H2/CO ratio might induce carbon formation (though the addition of water vapor ought to compensate).
- 2. The addition of water vapor might retard the rate of the F-T reaction, requiring a larger reactor.

An obvious fix, in case either of these hypotheses was later found to be a severe design limitation, would be to add a water gas shift step on a bypass portion of the feed gas upstream of the synthesis loop. This reactor could either use a sulfur resistant WGS catalyst upstream of the acid gas removal unit or use a conventional WGS catalyst downstream of acid gas removal. In the second alternative, CO_2 would be removed in a separate absorber using the same amine solution used for CO_2 removal within the loop. As a final alternative, of course, the CO_2 could be left

in the fresh feed gas, diluting the total feed to the F-T reactor and being removed in the downstream CO_2 absorber. The main problem with the first of these alternatives (sulfur resistant WGS) is that the H₂S going to the Claus Plant will be diluted with CO_2 .

6.1.1 Scoping Studies

Preliminary scoping studies have been performed to determine whether the aforementioned problems are real and the extent to which the baseline study costs might be in error if a pre-shift step is required. A joint effort was undertaken: We looked at possible retardation of the F-T reaction due to water vapor addition and MITRE made a preliminary estimate of the cost of adding upstream shift and CO₂ removal. Burns and Roe provided background information on the subject of carbon laydown.

The effect of water retardation is taken into account in the Viking slurry F-T reactor model by the use of the following rate equation (Anderson 1956):

 $\mathbf{r} = \mathbf{k} \cdot \mathbf{P}_{\mathbf{H}_2} \cdot \mathbf{P}_{\mathbf{CO}} / (\mathbf{P}_{\mathbf{CO}} + \mathbf{a} \cdot \mathbf{P}_{\mathbf{H}_2\mathbf{O}})$

Of course, in a slurry reactor, the partial pressures are replaced by the concentrations in the liquid phase. These are in turn related to the gas phase partial pressures by solubility and mass transfer relationships. When the concentration of water is low, the rate equation reduces to the expression used in Bechtel's slurry reactor model:

$r = k' \cdot C_{H_2}$

When water is the main byproduct, it is considered reasonable to use the simpler equation for conversions of up to 60% per pass. In a slurry reactor operating at low H_2/CO ratio, where CO_2 is the main byproduct, the simpler form should apply at even higher conversions than this. Whether added water vapor will change this conclusion depends on relative rates of reaction, gas solubilities and rates of diffusion - factors which can be tested using the Viking model.

As a starting point, five different material balances were set up around the F-T loop using the spreadsheet model described in the March quarterly report. The same H₂ conversion of 70.48% was used in each case and varying degrees of pre-shift and water addition were analyzed, trying to maintain the same CO conversion level by balancing the two. In some of the pre-shift cases CO_2 was removed from the feed gas; in other cases it was not. The five cases were as follows:

- 1. No pre-shift, balancing the F-T reactor by direct addition of water vapor supplementing the water vapor coming from the autothermal reformer via the recycle gas
- 2. Pre-shift to $0.5 H_2/CO$ ratio and CO_2 removal no water addition beyond that coming in with the recycle gas stream
- 3. Pre-shift to $0.5 \text{ H}_2/\text{CO}$ ratio without CO_2 removal no water addition beyond that coming in with the recycle gas stream
- 4. Pre-shift to $0.57 \text{ H}_2/\text{CO}$ ratio and CO_2 removal no water addition and water condensed out of the recycle stream
- 5. Pre-shift to 0.59 H₂/CO ratio without CO₂ removal no water addition and water condensed out of the recycle stream

The resulting F-T reactor feed gas compositions were then subjected to analysis by both the Viking and Bechtel reactor design models. The Bechtel model uses the final rate expression derived from Mobil pilot plant data as described in the March quarterly report. In both models, Bechtel's reaction stoichiometry was used in order to eliminate this as a variable. Slurry concentration was 22.5 wt% and inlet superficial velocity was 0.1 m/s. In both models it was found necessary to use a reactor length of 16 m to achieve the targeted 70.5% H₂ conversion. The results of all these calculations are summarized in Table 6-1 and the following conclusions can be drawn:

- There is some improvement in conversion level up to 3% when pre-shift and CO₂ removal are used.
- At the same time, the required number of 4.8 m diameter reactors is reduced by about 1 to 1.5 reactors out of a total of 23 to 24.
- When CO₂ is allowed to pass through to the F-T reactor, conversion per pass stays relatively constant and the number of required reactors increases by about 0.5 reactor.
- Total CO₂ rejected remains essentially constant.
- The two models show very similar trends, though the Viking model indicates a slightly greater improvement than the Bechtel model due to preshift. Nevertheless, one has to conclude that the effect of water retardation is small enough to be neglected.

• The hydrogen concentration in the recycle gas increases when pre-shift is used. This will improve the operation of the hydrogen recovery PSA unit.

While the two models give very similar results, Bechtel's analysis indicates that the Viking model uses expressions which give lower mass transfer rates and a faster rate of reaction. In addition, the Viking model includes dispersion coefficients for both gas and liquid phases, while Bechtel's model assumes gas phase plug flow and liquid phase fully backmixed. These effects apparently compensate one another.

Bechtel submitted Table 6-1 to MITRE, who did a preliminary economic analysis. The alternative chosen for study was to shift 20.4% of the raw gas stream, using 8,220 mph of steam, over a sulfur resistant shift catalyst, and then subject the entire gas to acid gas removal in a Selexol Unit. The resulting gas stream had a H₂/CO ratio of 0.511 and no water vapor was added to the F-T reactor. This was compared to a case with no pre-shift (0.388 H₂/CO ratio) and 6,000 mph of water vapor added to the F-T reactor. In a fax to Shelby Rogers dated 6/29/92, David Gray of MITRE concluded that the pre-shift case cost less than 1% more (\$14 million) and would add 1% to the cost of the gasoline/diesel produced.

On the subject of carbon formation, there is ample evidence from fixed bed studies that a low H_2/CO ratio is conducive to carbon laydown. Akgerman (Bechtel Slurry Reactor Design Studies) showed that a slurry reactor, because of differential gas solubility and mass transfer rates, should be less susceptible to carbon formation than a fixed-bed reactor. The key question, however, is the possible effect of water vapor in reversing carbon laydown as it does in steam reforming. John Marano, of Burns and Roe, has pointed out that, in the early 1960's, Kölbel and Engelhardt developed an alternative Fischer-Tropsch technology which reacted CO and H_2O in a ratio of 1:3. This work was done in both fixed-bed and slurry reactors. No mention was made of abnormal rates of carbon formation and this process represents the extreme in H_2/CO ratio, namely zero. From this, one must conclude that the addition of water vapor can indeed retard or eliminate carbon formation.

6.1.2 Recommendation for Basis of Design

The case without pre-shift has been the basis of design for the baseline case since the inception of the project and these scoping studies do not indicate any reason for change. It appears to be a viable case and is the lowest cost alternative. If, at a later date, evidence develops to show that pre-shift is a more suitable way to operate, then a change can be made at that time without affecting the economic conclusions to a significant extent.

6.2 ALTERNATE REFINING UPGRADE PROCESS (ZSM-5)

6.2.1 Alternative Case Design Basis

As was agreed on in the Project Kickoff Meeting, an alternative case design will be performed with ZSM-5 oligomerization as the primary upgrading step on the F-T reactor vapors. This configuration will duplicate the two-stage process piloted by Mobil for the DOE in the 1980's (see final reports under DE-AC22-80PC30022 and DE-AC22-83PC60019). In this configuration, all of the overhead vapor from the slurry F-T reactor is passed directly to a second stage, fixed-bed ZSM-5 reactor where olefins, oxygenates and heavy paraffins are converted to a mixture of isoparaffins, isolefins, naphthenes and aromatics. All of the oxygen atoms in the oxygenates are converted to H₂O byproduct. The C₅+ portion of this product is a quality gasoline and the light ends may be converted to gasoline by alkylation. The wax fraction is subjected to wax hydrocracking for distillates production. Mobil, in their design, also sent the C₃+ naphtha from the wax hydrocracker to the ZSM-5 reactor for upgrading. Yields were shown for the ZSM-5 product from this fraction, though the operation was not actually piloted.

6.2.2 Prediction of ZSM-5 Conversion and Yield

Preparatory to commencing this design, a method of predicting yields is necessary that gives results that are elementally balanced - or close to it - and that can be applied to different product distributions from the F-T first stage reactor. Rather than reanalyze the pilot plant data, Bechtel elected to perform a detailed analysis of the yields presented by Mobil for their low wax yield case (Tables 42 and 43 of their first report) and their high wax yield case (Tables VIII-2 and VIII-3 of their second report). A definite pattern was found in both conversion and yield, the two cases being quite similar:

- 1. A large portion of the 1-olefins and of the paraffins above C₇ were converted along with all of the oxygenates.
- 2. Isoparaffins, isoolefins, naphthenes and aromatics were formed.
- 3. There was no conversion of H_2 , CO, CO₂ or H_2O .
- 4. All of the oxygen atoms from the oxygenates ended up as H_2O .
- 5. The results were close to being in elemental balance.

Conversion and yield, by component, for Mobil's high wax (57% wax) and low wax (9% wax) cases were averaged by inspection. The resulting design factors and their application to the prediction of alternative case (two-stage) yields for the design 50 wt% wax yield case are shown in Table 6-2. While only the 50 wt% wax yield case is shown, these same design factors (highlighted in Table 6-2) may be used for any sensitivity case in 'he range of 10 to 75 wt% wax yield.

The way the calculation works is as follows:

- The percent conversion values, highlighted in the 5th column, are applied to the mols of stage 1 vapor after flashing, shown in the 4th column. This gives the mols converted, shown in the 6th column.
- The carbon distribution, shown in the 7th column, is applied to the total carbon converted shown at the bottom of column 6 as 13266.6 atoms of carbon per hour and the resulting atoms of carbon for each component are translated into mols and added to the first stage vapor less the mols of that component converted. The resulting second stage (ZSM-5) product is shown in the last column (column 8).
- There is no conversion of carbon dioxide, nitrogen, oxygen, carbon monoxide, hydrogen or water in the second stage. Water is produced to balance the atoms of oxygen present in the oxygenates from stage 1.
- As can be seen from the atom balances (shown at the bottom of columns 4 and 8), the second stage reactor is in elemental balance on carbon, oxygen and nitrogen and close to being in balance on hydrogen. A very slight increase (less than one decimal place) is the carbon distribution to one of the aromatics and a corresponding decrease in one of the paraffins would be sufficient to balance the calculation.
- The mols of isoparaffin and isoolefin shown in the first stage product were developed by assuming 5% iso's in the C₄'s and 10% iso's in the C₅'s and C₆'s. These values are approximate and were developed from an inspection of Mobil's overall pilot plant results. They are applied to both the olefin and paraffin components through C₆. Above C₆, all normal paraffin and all 1-olefin are assumed since they predominate and it is unnecessary to distinguish for design purposes.
- As can be seen, the front end of the ZSM-5 product is concentrated in isoparaffins and isoolefins. Further breakdown of the light isoparaffins and isoolefins is possible but will be very rough since the raw data are not entirely

complete or consistent. The heavy end of the ZSM-5 product is almost entirely aromatic. The concentration of benzene in the C₅₊ fraction is 1.1 wt% and the total concentration of aromatics is 28.4 wt%.

If naphtha from the wax hydrocracker is sent to the second stage reactor, the product distribution shown in the Appendix to Mobil's second report, Table ARD-II-12 is the only estimate available for the composition of the resulting ZSM-5 product. The quantity is prorated on wax make and the naphtha yield in the wax hydrocracker and added to that produced from the first stage vapor. On the other hand, the wax hydrocracker naphtha may well be a suitable product for blending purposes without further treatment. This will require further study.

Preliminary balances have been run around the synthesis loop for the baseline and alternate cases using Bechtel's spreadsheet model. Addition of the second stage has only a minor effect until the wax hydrocracker naphtha is added and this, in turn, affects mainly the liquid product yield. Some effect is also seen on the autothermal reformer, which sees more light hydrocarbons.

6.2.3 Recommendations

The next step will be to program the above calculation procedure into the ASPEN SP model for the F-T loop. This will be straightforward. The loop balances will then be refined using ASPEN, but the overall conclusions arrived at using the spreadsheet model are not expected to change

The result of the ASPEN loop calculation will be a detailed product breakdown for the gasoline, wax and light ends. From this, the distillation curve, gravity and PONA of the gasoline can be determined. The gasoline octane number, however, can best be gotten directly from Mobil's pilot plant results. Typical second stage gasoline octane is 92 RON, 82 MON clear. The light ends will be processed similarly to the baseline case although the balances will be entirely different and it may be possible to eliminate isomerization. Wax processing will, of course, be identical to the baseline design except that the small amount of "wax" in the F-T vapor will have been converted to gasoline in the second stage reactor rather than being recovered as hydrocracker feed.

6.2.4 Elemental Balance

While the synthesis loop will be elementally balanced, for both the baseline and alternative cases, there is no need to continue this balance through all of the downstream processing equipment (though it may be useful to continue it through

Section 6

the hydrotreaters in the baseline design to determine hydrogen consumption). Detailed componential distributions can be converted to distillation curves, gravities and molecular weights and used to estimate other properties useful in conventional refinery process equipment sizing calculations, process yield estimates and final product properties.

Table 6-1 Effect of Pre-Shift

Upstream Shift	No	Yes	Yes	Yes	Yes				
H2O Removal - Upstream	N/A	Yes	Yes	Yes	Yes				
H2O Removal - Loop	No	No	No	Yes	Yes				
-			Results of Lo	Results of Loop Simulation					
Feed Gas HZ/CO Ratio	0.389	0.50	0.50	0.57	0.59				
Steam to F-T Keactor	6000	0	0	0	0				
H2 Conv.	70.48	70.48	70.48	70.48	70.48				
CO Conv.	86.80	86.90	86.82	86 <i>.</i> 92	86.56				
Syngas Conv.	81.66	80.65	80,58	80.15	79,81				
U	0_373	0.499	0.501	0.569	0.589				
A Fred Car to CTReason	-0.5602	-0.5969	-0.5564	-0.6125	-0.5548				
CTUA	245		<i>(</i> 1)						
	3 1 3	726	634	731	736				
N7	3300	2001	13104	13/0	17611				
(n)	100751	9921	4337	4363	4434				
HT	100231	51044	31201	8/513	86/55				
120	17040	3877	4320	00010	62/20				
Total - #mph	167437	159401	170447	155777					
H2/CO Ratio	046	0.615	0.618	0.707	172700				
CO2 Removal smph	0.40	0.010	0.010	0.701	0.725				
Unstream	n	11567	n	15708	0				
Within Loop	57908	41576	52072	27002	E3100				
Total	57908	53003	53073	5750	20100				
%HZ in Gas to H2 Rec.	40.9	469	A6 0	33201 AQ 8	33190				
Purge Rate - #mph	4920	4790	4820	4720	499				
% N2 in Purse	194	700	10.20	1/00	4000				
O2 to Auto, Ref #mph	959	948	978	20.0	007				
H2O to AutoRef - #mph	6738	4120	6776	4575	1527				
Feed to AutoRef - smph	32647	37374	33034	33647	3007				
HC Product - #/hr	524305	523735	573800	575499	573476				
		•====	Results of Vik	ine Simulation	2000				
Reactor ID m	4.8	4.8	4.8	48	48				
Reactor Length - m	16	16	16	16	16				
Sup Veim/s	0.1	0.1	0.1	0.1	87				
Cat. Concn. %	225	22.5	22.5	22.5	225				
H2 Conv.	69.15	71.60	69.51	72.09	69.65				
CO Conv.	88.04	90.20	88.91	90.87	89.08				
Syngas Conv.	82.09	83.12	81.50	83.13	80.93				
U	0.36103	0.48813	0.48297	0.55618	0.56432				
A	-0.5839	-0.6078	-0.5647	-0.6216	-0.5625				
SV Nm3/hr.m3	275.2	2747	275.7	274.7	276.0				
GHSV Nm3/hr.kg	1.629	1.610	1.640	1.609	1.650				
5.YI Nm3 syngas/hr.m3	197.4	213.3	195.0	218.2	193.6				
SIYII kgHC/nr.m3	40.70	43.97	40.20	44.99	39.90				
Reactor ASect - mZ	18.19	18.10	18.10	18.10	18.10				
Des Gas Kate Nm3/s	20.17	20.02	20.29	20.03	20,39				
Uncorr. Gas Kate m3/s	1.8096	1.8096	1.8096	1.8096	1.8096				
1 - K	526.2	526.2	5Z6.2	526.2	526.2				
F - ann Managar Cao Data Martín	24	24	Z4	24	24				
CROTT. Gas Rate NIT3/5	22.54	22.54	22.54	22.54	22.54				
Tet Busine Fred Area	89.44	88.80	90.00	88.84	90.45				
Tet Basting Fred - Minph	16/433	158400	170662	155777	172708				
Torni Fred Nim2 (he	1554/	71850	7/412	70660	78340				
No. Passion	1/02106	1610353	1735013	158368/	1755813				
HT area mA7/Banch	23.63	24.34	23,75	21.96	Z3.92				
Instant Chit	2011	2855	2583	2846	2475				
	NO	165	Tes	Yes	Yes				
neo nemoval - Upstream	N/A	Yes	Yes	Yes	Yes				
Higo Hemoval - Loop	No	No	No	Yes	Yes				
			Results of Beck	htel Simulation					
Heador ID m	4.8	4.8	4.8	4.8	4,8				
Reactor Length - m	16	16	16	16	16				

Baseline Study F-T

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Table 6-1 (Continued) Effect of Pre-Shift

Sup Velm/s	0.1	0.1	0.1	0.1	0.1
Cat. Concn. %	22.5	22.5	22.5	22.5	225
H2 Conv.	70.02	71.45	69.54	71.92	69.22
CO Conv.	86.29	88.07	85.73	88.62	84.96
Syngas Conv.	81.17	81.74	79.54	81.74	78.37
Ū -	0.373	0.499	0.501	0.569	0.589
2	-0.5602	-0.5989	-0.5564	-0.6125	-0.5548
SV Nm3/hr_m3	273.9	273.9	273.9	273.9	274
CHSV Nei3/hr.kg	1.837	1.531	1.840	1.800	1.840
STYI Nm3 syngas/hr.m3	222.3	223.9	217.9	223.9	214.7
STY II kg HC/hr.m3	46.34	46.66	45.42	46.66	44.75
Reactor XSect - m2	18.10	18.10	18.10	18.10	18.10
Des Gas Rate Nm3/s	20.45	20.43	20.48	20.43	20.51
Uncorr. Gas Rate m3/s	1.810	1.610	1.810	1.810	1.810
т-к	526.2	526.2	526.2	526.2	526.2
P-atm	24	24	24	24	24
Uncorr. Gas Rate Nm3/s	22.54	22.54	22.54	22.54	72.54
% Flow Area	90.67	90.61	90,85	90.63	90.96
Tot. Reactor Feed - #mph	167433	158400	170652	155777	172708
Tot. Reactor Feed - kgmph	75947	71850	77412	70660	78340
Total Feed Ng3/hr	1702186	1610353	1735013	1583687	1755813
No. Reactors	23.13	21.90	23.53	21.53	23.75
No. Tubes/Reactor	1472	1482	1444	1482	1423
HT area - m^2/Reactor	2643	2661	2592	2661	2555

Component				F-T Vapor	%Coav	Mols Converted	C Distr.%	Mols Product
Methane	1	4	0	1285.47	0	0.00	02	1312.00
Ethane	2	6	0	96.86	0	0.00	01	103.49
Promana	4	:		36/72	40	155.09	00	232.63
Propeac	3	6	č	343.84	40	127.54	60	3/6.00
n-C4 Paraffia	4	10	ŏ	6.67		000	45	212 92
i-C4 Paraffin	- 4	10	ō	3.35	ā	000	114	381.45
a-Cé Olefin	- 4	8	0	254.73	40	101.89	00	152.64
HCA Olean	4	8	0	13.41	0	0.00	20	79.74
LCS Paratin	5	12	0	6245	0	0.00	35	155.32
n-C3 Olefin	5	10	ŏ	187.44		182.40	11.5	3120/
I-C3 Olefin	5	10	ō	20.83	0	0.00	67	19860
C5-Naphthene	5	10	Ó	0.00	30	0.00		7.96
»-Cé Paraffin	6	14	0	51.76	0	0.00	0.4	60.60
HC6 Partifica	6	14	0	575	0	0.00	7.0	160.53
		12	U O	155.32	99	153.77	<u>60</u>	155
C6 Naphthene	6	12	ŭ	000	30	000	1.6	52.54
Cé Aromatic	6	6	ō	0.00	ő	000	11	24.37
n-C7 Paraffin	7	16	0	57.09	3	1.71		55.38
+C7 Parallin	7	16	0	0.00	0	0.00	4.0	75.BI
n-C7 Olefin	2	14	0	133.21	75	99.91	20	33.30
C7 Nuchthese	7	14	0	0.00	0	0.00	10	18.95
C7 Aromatic	7		ň	000	40	000	21	39,50
n-CS Paraffin	8	18	ŏ	\$7.72		30.00		1653
I-Of Paraffin	8	18	ō	0.00	õ	0.00	1.8	29,65
n-Cli Olefin	8	16	Ó	110.18	75	82.64		27.55
I-Cli Olefin	8	16	0	0.00	0	0.00	17	28.19
C5 Naphthene	8	16	Ð	0.00	100	000	21	34.82
Ca Arometic B-Ca Paralita	ð	10	0	000	0	0.00	8.6	142.62
HC9 Paraffin	ģ	20	ŏ	000	83	33,14	11	585
p-C9 Olefla	9	18	ŏ	90.98	85	77.33	00 00	10.21
HC9 Olefin	9	15	0	0.00	Ū.	0.00	0.5	11.79
C9 Naphthene	9	18	0	0.00	100	0.00	0.5	11.79
C Aromatic	9	12	5	000	0	0.00	7.1	104.66
CIO Paraffin	10	2	0	32.14	100	3214	<u>ao</u>	000
n-C10 Ojefin	10	20	ŏ	74 98	100	74.08	0.2	265
+C10 Olefin	10	20	õ	0.00	100	0.00	12	265
CIO-Naphthene	10	20	Ō	0.00	200	0.00	01	133
C10-Aromatic	10	14	0	000	0	0.00	26	34.49
	11	24	0	26.40	100	26.40	00	0.00
	11	22	Ű	61.59	100	61.59	<u>ao</u>	000
Cl2-Paraffin	17	26	ŏ	21.60	100	2140	13	15.68
C12-Olefin	12	24	ō	50.40	100	50.40	60	000
C12-Aromatic	12	18	Ó	0.00	0	0.00	11	12.15
C12-Paraffun	13	25	0	17.58	100	17.58	60	000
	13	26	0	41.02	100	41.02	00	603
CLPATOMETE CLAPsesfin	13	20	0	0.00	0	000	07	7.14
Citolefin	14		ň	33.15	100	14.21	00	600
C14-Aromatic	14	22	õ	000	100	0.00	LU 03	784
C15-Paraffan	15	32	Ö	11.37	100	11.37		
C15-Okfin	15	30	0	26.54	100	26.54	20	0.00
Clé-Parafin Clé Obén	16	34	0	9.00	100	9.00	0 0	C 00
C17-Parafin	16	32 34	ů.	4199 700	100	20.99	00	000
C17-Olefia	17	34	ŏ	16.38	100	7412	40	000
CI&Paraffin	18	38	ŏ	5.40	100	5.40	<u></u>	0m
CLE-Olefia	18	36	Ó	12.59	100	12.59		000
CI9-Paraffia	19	40	0	3.93	100	3.93	00	0.00
C19-Olefin Wass	19		· · · · · ·	916	100	9.16	60	000
TT 4.5 Only in Vance	743	66LL/8	1231	3.02	100	3.02	E.0	000
Onvia HC	49941	3-07 11 578	1 1T	15858	100	63.07	00	000
Ony ia H2O	195	527	1.02	157 84	100	157.94		uud
αά	- 1	a	2	52989.68	0	0.00		57090 69
NZ	Ō	Ō	õ	4287.32	ō	0.00		6287.32

Table 6-2 Second Step Yield Prediction

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Task 3 - Engineering Design Criteria

Table 6-2 (Continued) Second Step Yield Prediction

Ci i i i i i i i i i i i i i i i i i i	0	D	2	0.00	0	0.00	00	000
0	1	0	1	13264.75	8	0.00		13244 75
H2	0	2	0	13564.62	٥	0.00		13544.62
HOD	0	2	1	2147.56	0	0.00	0	2578.67
Ten				90587.32274	3805	1915.363235	160	91466.43202
C approx				85256.0364	453(-1.3163	13266.59348	100	85256,0364
Hatters				73910,7735	93117.6326	27546.44142		70119.3866
O atome				121752.77	336.1	380.81 00677		121752.77
in atoms				8574.63014	0	0		8574.2014
lotal - V/hr				3166.572.66	644065.4533	193201.8452		3166768.62

Baseline Study F-T

Section 6

Project Management

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Section 7 Project Management

7.1 TASK 7 - PROJECT MANAGEMENT

The ASPEN/SP process simulation software was transferred to a new Compaq 486 personal computer. This will improve the productivity of our design effort with the simulation program. Per PETC's request, Bechtel prepared a work scope for a fixed-bed F-T reactor case. However, the value of this case study does not justify the estimated cost unless more recent fixed-bed F-T reactor performance data is available.

As of June 21, 1992, the baseline study is slightly underbudget because payment for the purchase of ASPEN/SP software has not been disbursed and the startups of several subtasks have been delayed. The overall project schedule status at the end of the reporting period is shown in Figure 7-1.

7.2 KEY PERSONNEL STAFFING REPORT

The key personnel staffing report for this reporting period (March 16, 1992 through June 21, 1992) as required by DOE/PETC is shown below:

Name	Function	% Time Spent(a)		
Bechtel				
Bruce D. Degen	Process Manager	14		
Charles R. Brown	Offsite Facilities	<mark>0</mark> (b)		
Gary Lucido	Cost Estimating	0(c)		
Samuel S. Tam	Project Manager	73		
Yang L. Cheng	Process Supervisor	79		
Amoco				
J. J. Nicoholas	Subcontract Manager	5		
S. S. Kramer	Process Model/Simulation	6		

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

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

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

Baseline Study F-T

DOE F1332.3 (11.84)

D PLAN A STATUS REPORT

FORM APPROVED OMB NO 1001.1400

1. TITLE Baseline Design/Economics for Advanced Fischer-Tropsch Technology			2. REPORTING PERIOD 6/25/92 to 6/21/92				3. IDENTIFICATION NUMBER DE-AC22-91PC90027				
4. PARTICIPANT NAME AND ADDRESS Bochtol Corporation 50 Beate Street San Francisco, CA 9410			05				5. START DATE 9/26/91 6. COMPLETION DATE 9/25/93				
7. ELEMENT CODE	8. REPORTING ELEMENT	PURATION FY 92 ONDJFMAAMJJJASONDJFMAMJJJASA							10. PERCENT a. Plan	COMPLETE b. Actual	
Task 1	Baseline Design	0 0					\bigtriangleup			41	40
Task 2	Economic Evaluation			E				7			
Task 3	Engineering Design Criteria					····	=			48	25
Task 4	Process Flowsheet Simulation Model							Z		15	3
Task 5	Sensitivity Studies						E				
Task 6	Documentation and Training								=	7	
Task 7	Project Management & Administration		2000 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200 - 200				,			35	35
000	Completion ASPEN/SP software delivered First progress meeting							_			
11. SIGNATURE OF PARTICIPANTS PROJECT MANAGER AND DATE Samuel S. Tam											

Figure 7-1 Overall Milestone Schedule (as of June 21, 1992)

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