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BASELINE DESIGN/ECONOMICS FOR ADVANCED FISCHER-TROPSCH TECHNOLOGY. QUARTERLY REPORT, OCTOBER--DECEMBER 1991

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U.S. Department of Energy Pittsburgh Energy Technology Center

Baseline Design/Economics for Advanced Fischer-Tropsch Technology

Contract No. DE-AC22-91PC90027

Quarterly Report

October – December 1991





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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 the advanced Fischer-Tropsch 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 Fischer-Tropsch (F-T) technology.
- Prepare the capital and operating costs for the baseline design.
- · Develop a process flowsheet 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 first quarterly progress report and covers the period of September 26, 1991 through December 22, 1991, which is the reporting period covered by the three already published monthly status reports.

The report consists of four sections:

- Introduction
- Summary
- Study Progress by Task
- Key Personnel Staffing Report

Section 2 Summary

This report summarizes the activities completed during the period September 26, 1991 through December 22, 1991 according to the tasks scheduled for the period, i.e., Tasks 1, 3, and 7.

In Task 1, Baseline Design and Alternates, the following activities were completed:

- Specifications were set for the design bituminous coal and an alternate subbituminous coal.
- Shell provided process design information for a 2000-ton-per-day Shell gasifier for the design bituminous coal.
- DOE consultants, Burns and Roe and Mitre Corporation, supplied input to support the process design basis.
- A preliminary process model for the Fischer-Tropsch (F-T) reaction loop was developed with the ASPEN/SP process simulator software.

In Task 3, Engineering Design Criteria, activity was initiated to support the process trade-off studies in Task 1. The work to date consists of:

- Assembling relevant information for review as potential project input.
- Selecting environmental criteria.
- Deciding to use a generic western mine-mouth location for the subbituminous case.
- Selecting high-purity oxygen and using CO₂ as a coal-feed carrier gas to minimize inert gas content in the F-T reaction loop.

In Task 7, Project Management and Administration, the following activities were completed.

- An agreement was reached with Shell Oil Development Company on the work scope and the work schedule for preparation of a gasification process design package.
- A project kickoff meeting was held at the Bechtel Office in October. Conference notes were prepared, approved, and distributed.
- A copy of ASPEN/SP simulation software was obtained through the DOE/PETC licensing agreement with Simulation Sciences, Inc.

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• A draft Project Management Plan was completed and reviewed by PETC. Incorporation of PETC's comments was started.

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Section 3 Study Progress by Task

To carry out this study efficiently, it has been divided into seven major tasks:

- Task 1: Establish the baseline design and alternates.
- Task 2: Evaluate baseline economics.
- Task 3: Develop engineering design criteria.
- Task 4: Develop a process flowsheet simulation (PFS) model.
- Task 5: Perform sensitivity studies using the PFS model.
- Task 6: Document the PFS model and develop a DOE training session on its use.
- Task 7: Ferform project management, technical coordination, and other miscellaneous support functions.

During the reporting period (September 26, 1991 through December 22, 1991), several activities were completed in Tasks 1, 3, and 7. These accomplishments are described below.

3.1 TASK 1 - BASELINE DESIGN AND ALTERNATES

Work during the reporting period was focused on the baseline design. The baseline design is a F-T synthesis facility, using slurry reactors operating in the high-wax mode, to produce LPG, diesel, gasoline, and distillate from synthesis gas that was produced in Shell gasifiers from 20,000 tons per day (tdp) of bituminous coal. An alternate case will be performed to assess the impact of subbituminous coal on the baseline design.

3.1.1 Coal Selection

Discussions were held with Shell to help set the design specifications for the two coal types to be investigated in the study.

Bituminous Coal. Shell concluded that Illinois No. 6 run-of-mine (ROM) coal was unacceptable as a feed to their gasifier because of its high ash content (over 20 wt % on an as-received basis). Since Illinois No. 6 coal from the Burning Star Mine is put through a washing step in which the ash content is reduced to 10.5 wt % before it is transported to current customers, Shell agreed that the washed coal is an acceptable feed stock for the Shell gasifier and it will be used as the design coal. The analysis of the washed coal is shown in Table 3-1. Because the coal will be washed before it is delivered to the gasification unit, there will be no coal cleaning facility within the F-T plant.

Item	As Rec'd	Dry	
Higher Heating Value, Btu/Ib (measured)	11,193	12,246	
Province Analysis us 9/			
Heisture			
Moisture	8.60	-	
ASI	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 10	
Chlorine	0.09	0.10	
Oxygen (by difference)	7.32	8.01	
Ash Mineral Analysis, wt % ash		L	
Silica	P4	80	
Alumina	19	20	
Ferric Oxide	17.60		
Sodium Oxide	0.50		
Potassium Oxide	2.00		
Calcium Oxide	6.30		
Magnesium Oxide	1.00		
	1.00		
Phosphorous Pentovide	1.00		
	0.20		
	2	.90	
Undetermined	0	.50	

 Table 3-1

 Bituminous Coal Analysis: Illineis No. 6 (Washed) (a)

(a) Source: Burning Star Mine

Subbituminous Coal. The statement of work specified that Wyodak ROM coal be used for the subbituminous feed coal. Although Shell has not performed gasification testing on Wyodak coal, they have tested the Buckskin subbituminous coal from Wyoming in their Texas pilot plant. Since the compositions of the Buckskin and the Wyodak coals are similar, the Wyodak coal will be used as the design subbituminous coal and the gasifier performance will be estimated by using the actual operating data from the Buckskin tests. The analyses of the Wyodak and Buckskin coals are shown in Table 3-2.

item	Wyoming Wyodak	Wyoming Buckskin
Higher Heating Value, Btu/lb (as received)	8,055	8,345
Proximate Analysis, wt % as received		
Moisture	31.0	28.77
Volatile Matter	30.1	34.33
Fixed Carbon	32.9	30.53
Ash	6.0	6.37
Tctal	100.0	100.0
Ultimate Analysis, wt % as received		
Carbon	46.81	51 22
Hydrogen	3.25	2.52
Nitrogen	0.65	0.77
Sulfur	0.4	0.86
Oxygen (by difference)	11.87	9.48
Chlorine	0.01	0.01
Ash	6.01	6.37
Moisture	31.0	28.77
Total	100.0	100.0

Table 3-2 Subbituminous Coal Analyses: Western ROM Coal(a)

(a) The design coal is Wyodak but the gasifier performance will be based on actual test data obtained with Buckskin.

3.1.2 Gasification Process Design

The Shell gasification process design will be based on the maximum gasifier size and will include:

- Shell gasifier
- Slag handling
- High temperature cooling/particulate removal
- Flyslag handling
- Gas treating and cooling (includes HCN/COS hydrolysis)
- Sour water stripping

The Shell process design package will include an overall material balance and utility requirements.

Shell has completed its design for a 2,000 tpd (single largest size) Shell gasifier processing the design bituminous coal, Illinois No. 6 washed coal. As specified by Bechtel, the design basis includes the use of high-purity oxygen (99.5 percent O_2) and the use of CO₂ (recovered from the acid gas removal unit) as a coal feed carrier gas.

The block flow diagram for the gasification plant for a single gasifier is shown in Figure 3-1. Table 3-3 shows the corresponding material balance.

3.1.3 Fischer-Tropsch Reactor Yield Correlations

Burns and Roe and Mitre Corporation, DOE consultants, provided comments pertaining to the F-T reactor yield correlations. This information will be incorporated, whenever applicable, to the final correlation of Mobil data on the F-T reactor yield.

Burns and Roe provided a paper on the formation and composition of the liquid phase in F-T reactors, a curve relating chain growth probability versus temperature with alpha values as a parameter, and a curve relating chain growth probability to weight percent wax production. The Mitre Corporation provided a block flow diagram and material balance for the recycle loop for the Shell-slurry F-T reactor with Wyoming coal.



Figure 3-1 Shell Gasification Plant Block Flow Diagram

Stream No. ^(b)	1	2	3	4
Stream Name	As Rec'd Coal Feed Ib/hr	Oxygen Feed moles/hr	Solid By-Product ib/hr	AGR Feed moles/hr
Gases:				
H ₂				3,243.7
co				9,037.6
CO2				593.3
H ₂ S/COS				140.2
NH3				trace
CH4				2.3
N ₂		20.9		95.2
H ₂ O				38.7
02		4,154.7		
HCN				trace
Liquids:				
H ₂ O			2,203	1
Solids:				
Coai	166,666			
Slag			18,200	
Sultur			265	
Total (lb/hr)	166,666	133.534	20,728	294,011

Table 3-3 Shell Gasification Plant Material Balance (a)

(a) Flow rates are for a single gasifier. The baseline design will require multiple gasifier units.(b) Refer to Figure 3-1 for stream numbers.

3.1.4 ASPEN/SP Modeling

Simulation Sciences, Inc. delivered a copy of the ASPEN/SP simulator to Bechtel. Amoco provided physical property information that they use in the input files of their direct liquefaction baseline study models. Bechtel used this physical property data to ensure internal consistency between the Amoco and Bechtel ASPEN/SP process models.

Amoco also specified the preliminary cost scaling parameters that the ASPEN/SP process FPS models will respond to. Bechtel will determine the parameter ranges for each of these process units as they apply to the F-T reaction loop.

3.2 TASK 3 - ENGINEERING DESIGN CRITERIA

Work on Task 3 was initiated during the reporting period to support the activities related to the baseline design case.

The environmental strategy developed for the Direct Coal Liquefaction Study (DE-AC22-90PC89857) was reviewed and determined to be applicable to the present study. It will be updated for different design philosophy, process selection, and potential pollutants.

After reviewing the level of effort involved, Bechtel determined that for the subbituminous coal alternate, the site location will be a generic western U.S. location at the mouth of a Wyodak coal mine. Bechtel will limit its process design efforts to those associated with coal composition (i.e., coal preparation and gas cleanup). The use of air cooling will be maximized for both the western and eastern cases.

Studies were conducted to determine how to minimize the inert nitrogen gas content in the F-T recycle gas loop. A typical design for a Shell gasification process for an integrated gasification combined cycle (IGCC) plant uses an air separation unit that produces an oxygen stream containing 95 percent oxygen. The unit also provides compressed nitrogen for coal pressurization and conveying to the gasifiers. An investigation showed that the benefits from the use of higher purity oxygen (99.5 percent vs 95 percent O_2) outweigh the increase in the air separation plant costs. Some of the key benefits are reduction of equipment size in the F-T reaction loop and lower energy requirement of the recycle gas compressors, the cryogenic unit, and the PSA unit. To further reduce the inert gas content in the F-T reaction loop, a highconcentration CO_2 stream from the acid gas removal units is used, instead of nitrogen in the coal feed system. These two changes were selected as design criteria and specified to Shell as part of the basis for the gasification plant design.

3.3 TASK 7 - PROJECT MANAGEMENT AND ADMINISTRATION

During the reporting period, the major activities in Task 7 were holding a kickoff meeting, preparing a draft Project Management Plan (PMP), and arranging for the use of ASPEN/SP software.

The kickoff meeting was held October 21, 1991 in Bechtel's San Francisco offices and attended by representations of PETC, Amoco, Bechtel, and Burns and Roe (consultants to PETC). The study's scope, goals, methodology, and schedule were reviewed with emphasis on a DOE list of "Areas of Interest and Questions to be Addressed" as follows:

- Design basis for the base case
- Product mix
- Methodology for selecting process alternatives
- · Selection of thermodynamic and physical property methods
- PFS model level of detail

The conclusions reached during the kickoff meeting were incorporated into a draft PMP. The PMP consists of five sections:

- Introduction
- Study Objectives
- Project Scope and Schedule
- Management Approach and Project Control
- Program Administration

The draft PMP was issued in November and reviewed by PETC. Their comments are being incorporated into a final document.

Bechtel has received a copy of ASPEN/SP simulation software through the DOE/PETC licensing agreement with Simulation Sciences, Inc. The ASPEN/SP software will be located at Bechtel for the duration of the project. Bechtel will use this software for process design work. The intent of using ASPEN/SP is to develop process data which may be incorporated directly into Amoco's process flowsheet simulation model.

The overall project schedule status at the end of the reporting period is shown in Figure 3-3.

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Figure 3-1 Overall Milestone Schedule (as of December 22, 1991)

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Section 4 Key Personnel Staffing Report

The key personnel staffing report for this reporting period (September 26, 1991 through December 22, 1991) as required by DOE/PETC is shown below.

Name	Function	% Time Spent ^(a)
Bechtel		
Bruce D. Degen	Process Manager	22
Charles R. Brown	Offsite Facilities	47
G. Lucido	Cost Estimating	0(p)
Samuel S. Tam	Project Manager	95

Amoco

A.	Schachtschneider	Subcontract Manager	8
S.	S. Kramer	Process Model/Simulation	8

- (a) Number of hours spent divided by the total available working hours in the period and expressed as a percentage.
- (b) G. Lucido of Bechtel did not spend any time in this reporting quarter because there was no cost estimating work required.

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