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March 30, 1993

U. S. Department of Energy
Pittsburgh Energy Technology Center
Mail Stop 922-H
P. O. Box 10940
Pittsburgh, PA 15236

Attention: Mr. Swenam Lee
Project Manager

Subject: D.O.E. Coal Liquefaction
Base Line Design and System Analysis
Contract No. DE-AC22 90PC89857
Bechtel Job No. 20952
Final Report on Baseline and Improved Baseline
Executive Summary
Letter No. BLD-142

Dear Mr. Lee:

Enclosed are three copies of the Executive Summary of the Final Report on the Baseline and the Improved Baseline and system analysis for the above contract. The final report is published in nine volumes and two volumes of appendices.

Copies of the Executive Summary to other members of DOE, as requested by the contract, are sent directly to each of them.

Please feel free to contact me should you have any questions.

Sincerely yours,

Syamal K. Poddar
Project Manager

SKP:tr

Enclosure

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The information and data contained in this report are the result of an ecomonic evaluation and a preliminary design effort and because of the nature of this work no guarantees or warranties of performance, workmanship, or otherwise are made, either expressed or by implication.

EXECUTIVE SUMMARY

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1. Introduction

This study is the result of a contract between the Pittsburgh Energy Technology Center (PETC) of the U.S. Department of Energy (DOE) and Bechtel with Amoco as subcontractor. The overall objective of the study was to develop a baseline and an improved baseline design of a conceptual direct coal liquefaction plant together with several processing options, the capital costs and economics for such a complex, and an ASPEN/SP based computer simulation model of the complex. Bechtel, with Amoco as team members, initiated the study on May 16, 1990.

During the course of the study the contract was modified several times. Primary modifications to the contract were to include 1) Naphtha reforming as an additional option to the baseline design and 2) study an improved baseline case by utilizing a different set of design parameters of the baseline liquefaction reactors. The new criteria was to increase the coal space velocity through the liquefaction reactor based on experimental data from the advanced coal liquefaction facility (pilot plant) at Wilsonville, Alabama. These data were published after the project was initiated.

As a result of these and other minor modifications, the completion date was extended to March 15, 1993.

2. Scope and Technical Approach

The scope of the study and the technical approach to accomplish the overall objectives of the study include:

- a baseline design to produce coal liquid for refining feed based on a specific Wilsonville pilot plant run which was deemed to represent the best available run with Illinois #6 coal, and other engineering evaluations,
- a cost estimate and economic analysis,
- a computer model incorporating the above two steps that is applicable over a wide range of capabilities and selected process alternatives,
- a comprehensive training program for USDOE/PETC staff to understand and use the computer model,
- a thorough documentation of all underlying assumptions for baseline design and baseline economics,
- a user manual and training material which will facilitate updating the model for the future, and
- expand the above objectives for the improved baseline case.

3. Management and Execution Philosophy

The project was managed via the concept of Configuration Management. The concept of Configuration Management was tailored to this study and was condensed into two fundamental control mechanisms, i.e., 1) Trend control and 2) Change control. Trend control is the system/procedure used to identify and document potential changes (Trends). Scope changes are the approved outcome of Trend control. By the Change control procedure, the scope change with associated cost and schedule impacts is incorporated in the project.

In order to carry out the study efficiently, the study was divided into seven major tasks with each task having several identifiable subtasks. In Task I the study was defined. The baseline and the improved baseline design were developed in Task II. The capital, operating and maintenance costs were developed in Task III. Mathematical models for computer simulation were formulated in Task IV. Development and validation of the model was conducted in Task V. Documentation of the process simulation and training program was conducted in Task VI. Whereas, the above mentioned six tasks are functional tasks, the remaining task, Task VII, was a task for project management, technical coordination and other miscellaneous support functions. Functional tasks (Tasks II through VI) were accomplished by a part time functional group while the project management and technical coordination were accomplished by a core management group (Task VII).

A set of procedures as prescribed by PETC together with relevant Bechtel's project procedures customized for this project were employed to achieve the project goals.

4. Deliverables

There are several deliverables for this study. The deliverables to DOE/PETC are grouped as follows:

- Monthly and quarterly progress reports
- Topical reports for each task (issued at the completion of each task)
- A stand-alone report for the improved baseline
- A multi-volume final report upon completion of the study
- ASPEN/SP process simulation documentation including basic assumptions for the process simulation
- An operating manual for models
- Comprehensive training program for the USDOE/PETC staff
- ASPEN/SP simulation software (limited license)

5. Baseline and Improved Baseline Designs

The basis for the design is a mine mouth plant located in southern Illinois. The feed coal is Illinois no. 6 (Burning Star mine) coal. The design basis, both the baseline design and the improved baseline design are based on experimental data generated at Advanced Coal Liquefaction Facility (pilot plant) located at Wilsonville, Alabama.

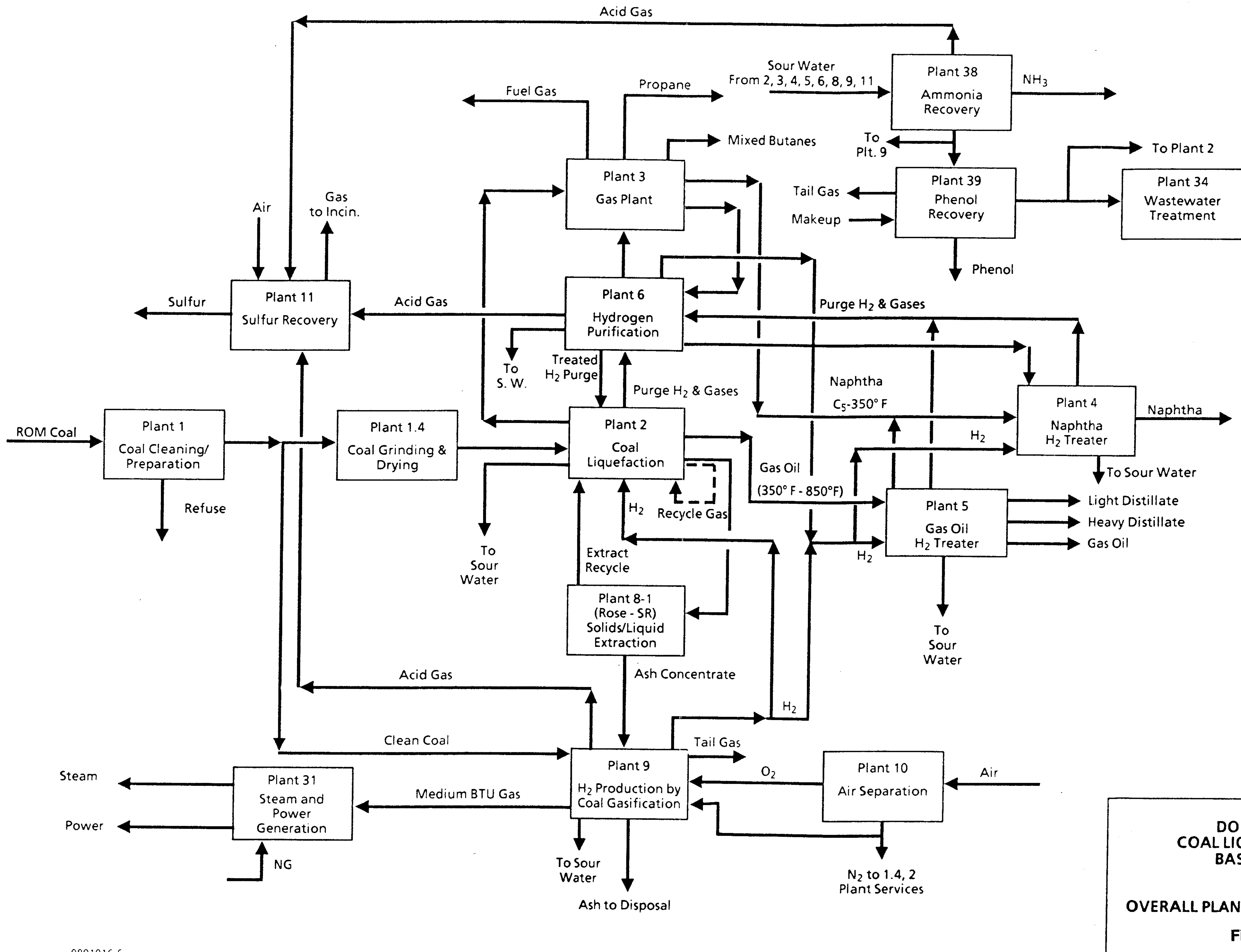
The commercial coal liquefaction complex for this study is comprised of a number of process plants supported by several off-site plants. The process plants which are designated as Inside Battery Limit (ISBL) plants are interconnected with the off-site plants designated as Outside Battery Limit (OSBL) plants.

The overall plant configuration for the coal liquefaction complex is the same for the baseline, as well as the improved baseline. The plant configuration is schematically shown by a simplified block flow diagram, Figure 1. This figure highlights the interconnections of primarily the ISBL plants.

Run of Mine coal enters the complex through the coal cleaning and handling plant (Plant #1), which is a Jig cleaning plant. Clean coal containing 11.47% ash (MF), upon further grinding and drying to a moisture level of 2 wt% (as is) in Plant 1.4, is fed to the liquefaction plant (Plant 2). The light products of Plant 2 are sent to the gas plant (Plant 3) to separate into fractions such as the fuel gas, propane and mixed butanes. The C_5-350°F stream goes to the Naphtha hydrotreater (Plant 4). The 350-850°F fraction from Plant 2 goes to the Gas Oil hydrotreater (Plant 5).

Required hydrogen for the complex is provided via coal gasification from Plant 9 which utilizes the Texaco technology. The coal liquefaction bottoms goes to Kerr McGee's ROSE-SR plant (Plant 8) which produces an extract that is recycled back to the liquefaction plant, and an ash concentrate stream that goes to the gasifier (Plant 9).

The hydrogen purged from Plant 2 is recovered by the hydrogen purification plant (Plant 6), which is a combination of membrane and PSA units. The treated hydrogen is recycled back to Plant 2. Sulfur is recovered by a sulfur recovery plant (Plant 11). Sour water collected from various plants is sent through the ammonia recovery plant (Plant 38). Part of this treated water is sent to the coal gasification plant and the rest to the phenol recovery plant (Plant 39) followed by a waste water treatment plant (Plant 34). The oxygen required by the coal gasifiers is supplied by the air separation plant (Plant 10).



DOE / PETC
COAL LIQUEFACTION
BASE CASE

OVERALL PLANT CONFIGURATION

Figure 1

The most important process plant in the entire complex, often referred to as the "heart of the complex" is the coal liquefaction plant, Plant 2. The Plant 2 design for the baseline was developed by HRI, Inc.; whereas for the improved baseline case the Plant 2 design was developed by the Amoco/Bechtel team. The design is for a close-coupled, catalytic-catalytic, two stage coal liquefaction (H-COAL by HRI) plant with extract recycled from the critical solvent deashing (ROSE-SR) plant.

The key operating conditions, overall product yields and design data for the baseline design as well as for the improved baseline design are shown in Tables 1 through 3.

As shown in Table 1, the coal space velocity (lb MAF coal/hr/lb catalyst) for the improved baseline is higher than the baseline, 1.95 vs. 1.12 respectively.

Table 1
Key Operating Conditions

	257-J	Improved Baseline	Baseline
Coal SV, lb MAF/hr/lb Cat	2.17	1.95	1.12
Temp., °F Reactor I Reactor II	 809 760	 810 760	 790 760
Catalyst addition, lbs/ton MF coal each stage	3/1.5	3/1.5	3/1.5
Solvent/MAF Coal	2.25	2.26	2.46
Resid in Solvent, wt%	50	50	50

It is apparent from Table 2 that the gas (C_1 - C_3) make is slightly higher for the improved baseline; whereas the $C4^+$ liquids are the same for both cases. The hydrogen consumption is slightly higher for the improved baseline.

Table 2
Overall Product Yields

Yields, wt% MAF	257-J	Improved Baseline	Baseline
H2S + H2O + COx + NH3	15.1	13.9	14.0
C1 - C3	5.4	5.5	4.8
(C4 - 350)°F (350 - 450)°F	14.5 7.1	15.8 7.3	16.9 7.5
(450 - 850)°F	44.2	48.1	46.8
$C4^+$ liquids	65.8	71.2	71.2
Resid	1.2	0.0	0.0
Organics in ash-conc.	18.5	15.7*	16.3
H2	(6.0)	(6.3)	(6.2)

* Run 261-F/G: 15.6%

As shown in Table 3 for the liquefaction plant, Plant 2, there are 4 operating trains for the improved baseline as compared to 5 trains for the baseline case. Also, for the improved baseline, the coal feed rate through the liquefaction reactor is about 9% higher than for the baseline case.

Table 3
Comparative Design Data: Improved Baseline vs. Baseline Designs

Design Cases	Improved Baseline		Baseline	
Number of Operating Trains	4		5	
Coal feed rate/train, Mlb MAF/hr	343.8		252.3	
Reactor [a,b]	1st Stage	2nd Stage	1st Stage	2nd Stage
Velocity, fps [c]				
Gas	0.14	0.19	0.11	0.21
Liquid	0.12	0.11	0.10	0.08
Bed Height, ft. [c]				
Settled	34	34	44	44
Expanded	77	77	77	77
Recycle/Fresh Feed ratio	5.6	3.1	6.0	3.3
Reactor Average Temp, °F	810	760	790	760
Bed Exotherm, °F	34	30	30	27
Reactor Outlet Temp, °F	827	775	805	774
H2 partial pressure, psia	2232	1934	2243	2061

(a) Catalyst: average diameter, 0.083 inches; length, 0.24 inches
(b) Reactor ID (excluding refractory), ft: 15
Refractory thickness, in.: 6
Total height, ft.: 85
Weight, Short tons: 1295
(c) Estimate based on kinetic model predictions.

The coal liquefaction complex is designed to produce approximately 60,000 barrels per day of C5+ hydrocarbon products. The primary products of such a complex are C3, C4, C5-350°F (Naphtha), 350-450°F (Light Distillate), 450-650°F (Heavy Distillate) and 650-850°F (Gas Oil). Besides these, there are three by-products from the plant. They are: 1) Ammonia, 2) Sulfur and 3) Phenols. Naphtha, Distillates and Gas Oil are hydrotreated to improve the stability of these products for storage and transportation.

The hydrocarbon product and by-product yields for the baseline and the improved baseline are shown in Table 4.

Table 4
Hydrocarbon Product Yields and By-product Yields for Baseline and Improved Baseline

Hydrocarbon Product Yields		
	Baseline	**Improved Baseline**
Coal Feed Rate (MAF) TPSD	15,140	16,503
<u>Component (BPSD)</u>		
Propane	4,407	3,884
Mixed Butanes	3,541	2,230
Naphtha	19,195	18,519
Light Distillate	7,803	7,403
Heavy Distillate	21,635	27,590
Gas Oil	13,310	21,370
Total	69,891	80,996
By-product Yields		
<u>Component (STPD)</u>		
Sulfur	740	859
Ammonia	244	277
Phenols	32	39

6. Designs for Various Options

Six options to the baseline design were evaluated as shown in Table 5. In addition, a seventh option was included where a naphtha reformer was integrated into the naphtha upgrading scheme.

For the improved baseline design case, only one option was considered, the lowest capital cost option.

The methodology utilized to select the options is explained below:

- Identify the primary process features and variables related to each process feature
- Define the baseline design by selecting the agreed upon combination of process variables/features
- Define each option by changing the variable of one process feature at a time, while maintaining the variables of other process features unchanged
- Combine the newly defined process features to define the respective option

Table 5
Process Features and Related Variables for Various Options

Process Features	Variables	Baseline	Option Number
Coal Cleaning Method	• Jig • Heavy Media Separation • Spherical Agglomeration	X	 1 2
Reactor Configuration	• Catalytic-Catalytic • Thermal-Catalytic • Catalytic-Catalytic with Vent Gas Separator	X	 3 4
Vacuum Bottoms Processing	• ROSE-SR • Fluid Coking [(1)]	X	 5
Hydrogen Production	• Coal Gasification (Texaco Technology) • Steam reforming of Natural Gas [(2)]	X	 6

(1) Coke from Coker is fed to Gasifier
(2) In this option the ash concentrate from the ROSE-SR unit goes to a fluid bed combustion unit

7. Capital Cost Estimates

7.1 Methodology for Capital Cost Estimates

The overall plant cost was estimated by developing the cost estimates (field cost) of each Inside Battery Limit (ISBL) plant and each Outside Battery Limit (OSBL) plant. For each plant (ISBL, as well as OSBL) the total field costs were estimated by summing the estimated costs of: 1) major equipment, 2) bulk materials, 3) subcontracts, 4) direct labor and 5) distributables (indirect costs).

The Nth plant (the concept of which is defined in this section) installed plant costs for the baseline case were calculated by 1) taking the estimated ISBL plant cost for each ISBL plant, 2) adding the respective proportional amount of total OSBL costs, and then 3) adding the proportional amount of home offices, engineering fee and contingency.

The Nth plant is defined as the Nth commercial plant built when the technology basis, plant design and operation are well established. The Nth plant has the following characteristics:

- Lowest reasonable plant cost contingency
- No spare trains
- Lowest reasonable engineering cost
- Shortest possible project schedule for construction and start-up
- Matured technology allowing the overall stream factor of the complex to be same as that of the First plant.

7.2 Capital Cost for Baseline

The capital costs estimates for the baseline design that were generated by following the above methodology are shown in Table 6 below. These estimates, as discussed earlier, are for the "Nth plant".

Table 6 Nth Plant Capital Cost for the Complex Baseline				
Plant #	No. of Trains	ISBL Plant Field Costs 1000$	ISBL Plant Adj. with OSBL Costs 1000$	Installed Plant Costs 1000$
1	5	91,000	131,000	160,800
1.4	10	87,500	126,000	154,600
2	5	932,200	1343,000	1,647,800
3	1	25,300	36,400	44,700
4	1	15,600	22,500	27,600
5	1	74,000	106,500	130,700
6	1	152,600	220,000	269,800
8	1	42,200	60,800	74,600
9	5	263,700	380,000	465,900
10	5	191,000	275,000	337,700
11	4	46,700	67,200	82,500
38	1	40,100	57,800	71,000
39	1	13,300	19,200	23,500
Total		**1,975,200**	**2,845,400**	**3,491,200**

7.3 Capital Costs for Options to Baseline

Overall Capital Costs (Nth plant) for Options

Following the same methodology as described above the capital cost estimates for all seven options were developed. These results are shown in Table 7. The lowest capital cost is for option 6 where hydrogen is produced by natural gas reforming. This option also was considered for the improved baseline design case.

Table 7 Nth Plant Capital Costs for the Complex for Options		
Op. No.	Option Description	Capital Costs $ Million
1	Liquefaction Feed Coal Cleaning by Heavy Media Separation	3,293.2
2	Liquefaction Feed Coal Cleaning by Spherical Agglomeration	3,552.3
3	Thermal-Catalytic Liquefaction Reactor Configuration	3,427.0
4	Catalytic-Catalytic Reactor Configuration with Vent Gas Separation	3,326.7
5	Fluid Coking of Vacuum Bottoms	3,308.0
6	Stream Reforming of Natural Gas plus FBC* Unit for Hydrogen Production	2,782.7
7	Naphtha Reforming	3,345.8

* Fluid Bed Combustion

7.4 Capital Costs for Improved Baseline

Installed plant costs for the complex were calculated by 1) taking the estimated ISBL plant cost for each ISBL plant, 2) adding the respective proportional amount of total OSBL costs and then 3) adding the proportional amount of home offices, engineering fee and contingency. The results are shown in Table 8. This table also includes the number of trains (operating and total number) for each plant. Because the cost estimates are for the "Nth plant" scenario, the number of operating trains and the total number of trains for any ISBL plant are the same.

Table 8 Nth Plant Capital Costs for the Complex Improved Baseline					
Plant #	No. of Oper. Trains	Total No. of Trains	ISBL Plant Field Costs 1000$	ISBL Plant Cost Adj. with OSBL Costs 1000$	Installed Plant Costs 1000$
1	6	6	104,900	1,571,700	182,000
1.4	12	12	96,800	140,000	171,800
2	4	4	854,800	1,236,400	1,517,000
3	1	1	23,600	34,100	41,900
4	1	1	13,600	19,700	24,100
5	1	1	82,900	119,900	147,100
6	1	1	130,000	188,000	230,700
8	1	1	41,700	60,300	74,000
9	6	6	303,300	438,700	538,200
10	6	6	222,500	321,800	394,800
11	5	5	55,100	79,700	97,800
38	1	1	45,000	65,100	79,900
39	1	1	16,000	23,100	28,400
Total			**1,990,200**	**2,878,500**	**3,531,900**

7.5 Capital Costs for Option to Improved Baseline

The total installed cost for this option was re-estimated from the baseline estimates by replacing the cost of the directly affected baseline plant with the cost of the optional plant. All other cost modifications impacting the indirectly affected plants were done using the cost vs. capacity correlations.

Thus the installed costs reported in the last column of Table 9 for the Nth plant scenario are those for the entire complex with hydrogen production by steam reforming of natural gas (Option 6).

For this option the directly affected plants are hydrogen production by coal gasification (plant 9), air separation plant (plant 10), and the additional fluid bed combustion (FBC) unit in plant 31.4-01 for processing the ROSE-SR bottoms. For this option, as discussed earlier, the air separation plant (plant 10) is not a part of this complex.

Table 9
Nth Plant Capital Costs for the Complex
Improved Baseline with H2 Produced by Natural Gas Reforming

Plant #	No. of Oper. Trains	Total No. of Trains	ISBL Plant Field Costs 1000$	ISBL Plant Cost Adj. with OSBL Costs 1000$	Installed Plant Costs 1000$
1	6	6	86,000	115,800	142,100
1.4	12	12	96,800	130,400	160,000
2	4	4	854,800	1,151,300	1,412,600
3	1	1	23,600	31,700	38,900
4	1	1	13,600	18,300	22,500
5	1	1	82,900	111,700	137,000
6	1	1	129,900	174,900	214,700
8	1	1	41,700	56,200	68,900
9-01	3	3	224,700	302,600	371,300
11	5	5	33,700	45,400	55,700
38	1	1	42,500	57,300	70,300
39	1	1	18,500	24,900	30,500
Total			**1,648,700**	**2,220,500**	**2,724,500**

8.0 Modeling Tools

The complete modeling package that was developed under this project was designed to be a research guidance tool to study technology advances and options in a case study approach. It does not feature optimization capabilities and is not a detailed process design tool. It was designed to predict the effects of various process and operations changes on the overall plant material and utility balances. It also was designed to predict the effects on the capital cost and operating labor. The modeling tools were developed in a way so that they are applicable for the baseline as well as for the improved baseline cases.

A separate LOTUS spreadsheet economics model was developed that does a discounted cash flow analysis of the project taking results directly from the process simulation model output to calculate project economics.

Figure 2 shows a simplified user input-output diagram of the various computer models used in this project, and how they interact with each other. The ASPEN/SP process simulation model is the heart of the modeling system. Although this model resides in a detailed process simulation model, many simplifying assumptions and approximations were made to keep the model manageable and still satisfy the requirements of being a research guidance tool, and not a design tool. If detailed process simulation models for design were developed, the system would have become unmanageable and would have required excessive computer facilities.

The ASPEN/SP process simulation model is based on the detailed plant designs developed for the baseline design and improved baseline design. Fortran user block models are used to simulate most of the plant, and to predict their utilities consumptions, labor requirements and capital costs. Results are available in several forms including the normal ASPEN/SP reports, specific plant summary reports, and an overall management summary report. A small output file also is generated for transferring the key process simulation model results to the LOTUS spreadsheet economics model.

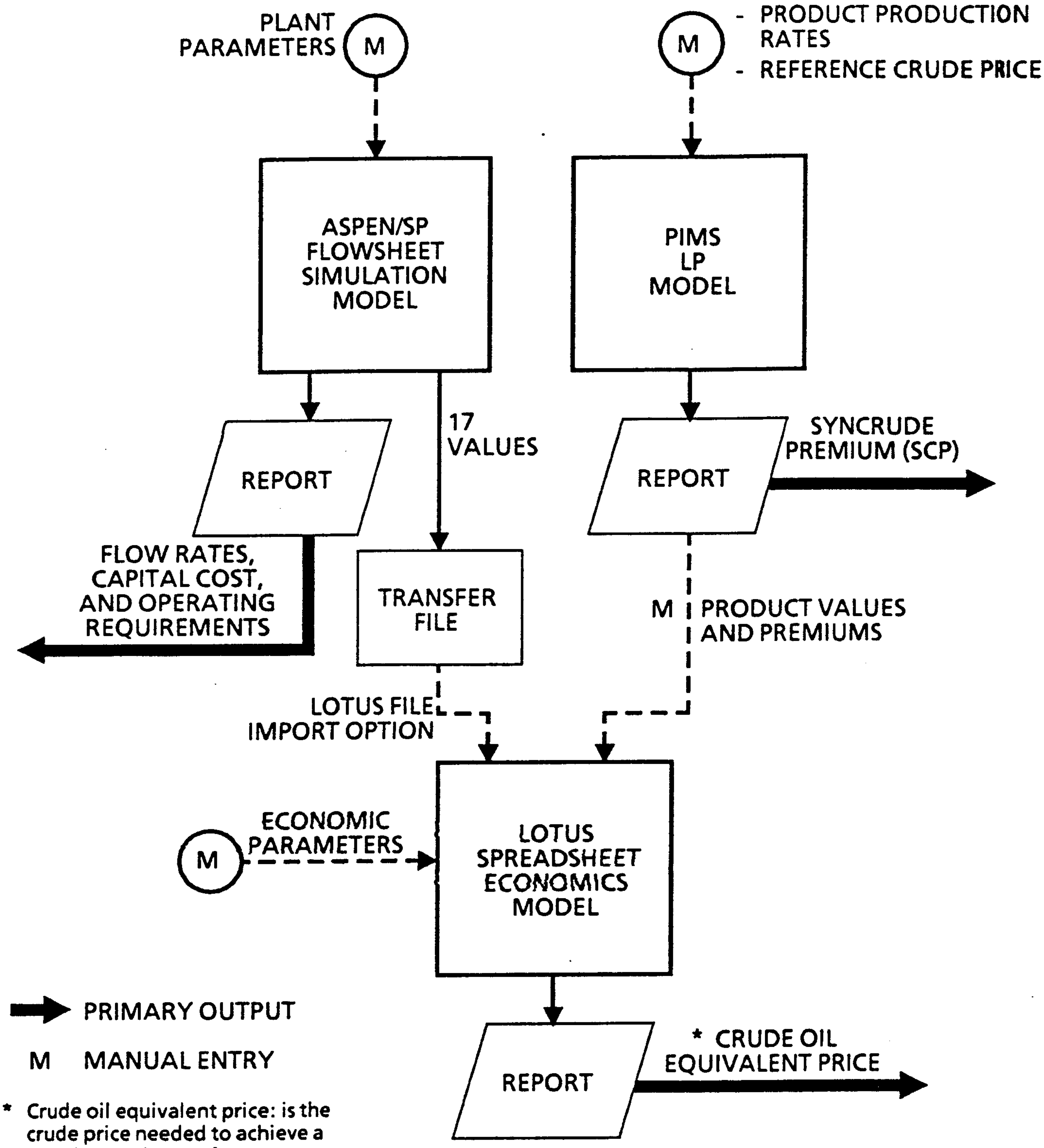
Bechtel's linear programming tool, PIMS (Process Industry Modeling Systems) was used to develop the valuation of coal liquid products by simulating a typical PADD II (mid-western) refinery. The product valuation expressed as Syncrude premiums was used for the LOTUS spreadsheet economics model. The product valuations were calculated for various scenarios as case studies. For these scenarios, different percentages of coal liquid products were assumed to be fed into the refinery with corresponding amounts of petroleum feed being backed out. In general, it was assumed that the naphtha faction of the coal liquid (C_5 - 350) was sent to the reforming unit, the light distillate fraction (350-450) was for blending (diesel and fuel oil), the heavy distillate fraction (450-650) was for diesel and fuel oil blending and also used as Fluid Catalytic Cracking Unit (FCCU) feed, and the vacuum gas oil (650-850) was used as fuel oil blending stock and FCCU feed.

The LOTUS spreadsheet economics model takes the results from the other two models along with user supplied economic parameters and does a complete discounted cash flow analysis. This spreadsheet will generate the net present value of the project at a specified internal rate of return (IRR) on equity. It also can be used to calculate what crude oil price is required to obtain a specific internal rate of return. In addition, this spreadsheet model allows studying the effects of other economic assumptions on project economics.

The basic process simulation model developed under this project simulates the baseline design. Seven optional cases also were simulated. These optional cases were simulated either by minor modifications to the basic ASPEN/SP input file, or by the use of a separate, but similar ASPEN/SP input file. The separate input files are required because some cases have a different flowsheet logic which could not be blended into the basic simulation model input file.

Figure 2

SIMPLIFIED USER INPUT - OUTPUT DIAGRAM
FOR COMPUTER MODELS USED IN DIRECT COAL LIQUEFACTION STUDY



* Crude oil equivalent price: is the crude price needed to achieve a 15% internal rate of return.

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9.0 Overall Product and By-product Valuation

Product Valuation

The coal liquid products were valued by utilizing Bechtel's linear programming modeling tool, PIMS (Process Industry Modeling Systems). A typical PADD II refinery configuration and crude mix with a fixed price were assumed. Also, it was assumed that the coal liquid naphtha (C5-350°F) was sent to a reforming unit, the light distillate (350-450°F) was used for blending (diesel and fuel oil), the heavy distillate (450-650°F) was used for diesel and fuel oil blending or as FCCU feed, and the vacuum gas oil (650-850°F) was used as fuel oil blending stock and FCCU feed. The product valuation was then determined for various scenarios and expressed as "Syn-Crude Premium" (SCP). The SCPs varied between 1.07 and 1.27.

By-product Valuation

The by-products for this complex are sulfur, ammonia, phenol, propane and mixed butanes. The production rate of these streams for the improved baseline case and their assumed respective prices are shown below in Table 10.

Table 10

By-product Values

	Production Rate	Price
Sulfur	858.8 STPD	$80/ton
Ammonia	276.6 STPD	$120/ton
Phenol	38.5 STPD	$400/ton
Propane	3884 BPSD	$7.50/bbl
Mixed Butanes	2230 BPSD	$14.50/bbl

10. Economics and Sensitivities

The economic analysis to determine the Crude Oil Equivalent price (COE) in $/bbl was carried out using the LOTUS 1-2-3 based spreadsheet model developed by Amoco. There were several key assumptions made in carrying out this analysis. These key assumptions are listed below.

Key Assumptions

Years of construction	4
Years of operation	25
Depreciation, Years	10
Maintenance, % initial capital	1
Working capital, % revenue	10
Working capital, % liquid	50
Owner's cost, % initial capital first year operation	5
Bank interest rate	8
Federal income tax rate, %	34
Percent equity	25
Percent IRR* on equity	15
General inflation %	3
Raw material price escalation	same as general inflation of 3%
State Tax	0
SCP	1.07

* IRR is the internal rate of return

Economic Results

The results of the economic analysis are presented in Table 11. These results are based on capital cost estimates at mid 1991 and the project start date is six months later. The results are expressed in terms of Crude Oil Equivalent (COE). They were obtained at 15% IRR on equity. Results thus obtained are summarized for four cases. These cases are 1) baseline design, 2) Improved baseline design, 3) baseline design with hydrogen produced by gas reforming, and 4) improved baseline with hydrogen produced by natural gas reforming. As shown in this table, the best economic case studied in this project is the improved baseline case with hydrogen production by natural gas reforming.

Table 11
Results on Economics

Case	COE $/bbl
Baseline	38.55
Improved Baseline	33.45
Baseline with H2 from Natural Gas	36.00
Improved Baseline with H2 Production by Natural Gas Reforming	31.00

Sensitivity on Economics

The economics sensitivity analysis was carried out to determine the impact of changes in capital, raw material pricing, owner's equity, price escalation (per EIA) on coal, natural gas and crude oil, and syncrude premium, respectively.

Results of the sensitivity analysis are shown in Tables 12 and 13. Table 12 presents the results on sensitivity analysis for the baseline whereas Table 13 shows similar results for the improved baseline.

As shown in these two tables for the baseline case, a change in capital cost by 10% changes the Crude Oil Equivalent price by $2.35/bbl, and a 25% change causes a change of $5.90/bbl in the Crude Oil Equivalent price. For the improved baseline case, similar changes cause the Crude Oil Equivalent prices to change by 1.95/bbl and $4.95/bbl respectively. A 25% change in coal and natural gas price individually changes the equivalent crude price by $2.30/bbl and $0.65/bbl, respectively, for the baseline, and $2.10/bbl and $0.55/bbl for the improved baseline.

Increasing the owner's equity by 100% (a change from 25% to 50% equity) increases the Crude Oil Equivalent price by $3.05/bbl for both cases.

When coal, natural gas and crude oil are individually allowed to escalate per the EIA forecast, instead of at the fixed rate of 3% (inflation), the equivalent crude oil price decreases by $8.70/bbl and $7.45/bbl for the baseline and the improved baseline, respectively. The increase in syncrude premium to 1.27 results in a drop of the Crude Oil Equivalent price by $6.15/bbl and $5.35/bbl, respectively.

Table 12

Sensitivities on Economic Results for Baseline

ECONOMICS	
Case	**COE $/bbl**
Baseline	38.55
Baseline with H_2 production from natural gas	36.00

SENSITIVITIES		
Item	**Change**	**Δ $/bbl**
• Capital	± 10% ± 25%	± 2.35 ± 5.90
• Raw Material		
Coal	± 25%	± 2.30
Natural Gas	± 25%	± 0.65
• Owner's Equity	± 100%	± 3.65
• Liquid yields	± 10%	- 3.50
• Price Escalation, per EIA		- 8.70
Coal	+ 1.6	
Natural gas	+ 3.5	
Crude oil	+ 2.9	
• Syncrude Premium	+20%	- 6.15

Table 13

Sensitivities on Economic Results for Improved Baseline

ECONOMICS	
Case	**COE \$/bbl**
Improved Baseline	33.45
Improved Baseline with H_2 production from natural gas	31.00

SENSITIVITIES		
Item	**Change**	**Δ \$/bbl**
• Capital	± 10% ± 25%	± 1.95 ± 4.95
• Raw Material		
Coal	± 25%	± 2.10
Natural Gas	± 25%	± 0.55
• Owner's Equity	± 100%	± 3.05
• Price Escalation, per EIA		
Coal	+1.6	- 7.45
Natural Gas	+3.5	
Crude oil	+2.9	
• Syncrude Premium	+0.20	- 5.35

11. Discussion

The engineering design, capital cost estimates and economics results presented in this report are all subject to the scope and constraints of the study, and the assumptions that were made during execution of this study. This section discusses some of these assumptions and limitations and comments on their implications.

Baseline Design Basis:

The baseline design basis is based on the then available pilot plant run data generated at Wilsonville pilot plant facilities (run 257E). This run was deemed to represent the best reliable run with Illinois No. 6 coal.

Improved Baseline Design Basis:

While the baseline study was at the final stage of completion a separate set of data became available which are for a relatively higher space velocity through the liquefaction reactors. These data are based on Wilsonville run numbers 257J, 261B and 261D. In light of these data, the baseline design basis appeared to be rather conservative. Because of the potential favorable economic impact of the higher space velocity, a separate case was studied, and it was designated as the improved baseline design case. The key design basis assumptions for the improved baseline were developed jointly by DOE/PETC, Amoco, Bechtel, and Burns and Roe Services Corporation by utilizing collective experiences and the available data based on the experimental runs mentioned above.

Nth Plant and Related Assumptions:

The concept of an Nth plant assumes that the technology for the direct liquefaction of coal is a mature one, and that there are numerous other plants already constructed and operating. Hence, it assumes that the engineering and construction of such a plant is achievable with minimal engineering and contingency costs and with short construction time. Furthermore, based on the collective operating and turnaround experiences and the same level of overall operating factor as the first plant (with spares), an immediate start-up would be achievable.

Selection of Technology for Coal Gasification for Hydrogen Production:

Two coal gasification technologies, the Texaco and Shell processes were evaluated for synthesis gas production for hydrogen production. Based on this evaluation it was concluded that for high pressure hydrogen production, Texaco's gasification process has lower capital and utility costs. Besides, it has been demonstrated that Texaco's gasifier can process H-coal liquefaction vacuum tower bottoms as well as ROSE-SR ash concentrate. Therefore, Texaco gasification technology was selected.

Producing electricity on site vs. importing power:

The conceptual design of the liquefaction complex considered having the power plant as a part of OSBL plants to make the complex self sufficient in power. The preliminary cost comparison between the option of producing power on-site vs. purchased power indicated that there was no special economic driving force for either option. On the other hand, having the power plant in-house provides self sufficiency in the availability of power. Therefore, on-site power generation was selected.

Syncrude Premium Factor:

The syncrude premium factor (SCP) which relates the coal liquefaction plant product values to a typical crude oil in PADD II refinery was determined in a rigorous manner using Bechtel's proprietary linear programming (LP) software refinery model (PIMS). A low SCP value of 1.07 was determined by forcing the refinery to make the same product slate that it would make on its typical crude oil feed, and another higher value of 1.27 was obtained by allowing the product slate to float to maximize profit. Since all refineries are different, the coal liquefaction product will have different values to different refineries, depending upon their internal processing configuration, location, product demands and business conditions. For the Nth plant scenario, the other operating coal liquefaction plants will be supplying a significant portion of the regional refinery feed. This would suggest that the lower SCP should be more realistic.

Options:

In addition to the baseline design case seven alternative processing options were studied. These seven alternative processing options are:

1. Liquefaction feed coal cleaning (to 8.6 wt% ash) by heavy media separation
2. Liquefaction feed coal cleaning (to 3.8 wt% ash) by spherical agglomeration
3. Thermal-catalytic liquefaction reactor configuration
4. Catalytic-catalytic liquefaction reactor configuration with inter-reactor vent gas separation
5. Fluid coking of the coal liquefaction vacuum bottoms.
6. Hydrogen production by steam reforming of natural gas with a fluidized bed combustor for ROSE-SR bottoms and thereby generating electric power
7. Addition of reformer for the naphtha product

Because the original baseline design with option 6 showed the lowest capital cost of the seven options, option 6 was studied with the improved baseline design case.

Models:

During this study, four models were developed to provide DOE with some additional tools for evaluating the benefits of direct coal liquefaction research and provide guidance for further research. These models are:

1. PIMS LP model of a typical PADD II refinery
2. Process simulation model of the entire coal liquefaction complex using ASPEN/SP software.
3. Lotus 123 spreadsheet economics model
4. Kinetic coal liquefaction rector model using ASPEN/SP software

The model of a typical PADD II refinery using PIMS LP software was developed to determine the valuation of the as-produced coal liquids. However, it obviously can be used for a similar purpose in other studies, and to study various effects on the domestic oil refining system.

The ASPEN/SP process simulation model of the entire coal liquefaction facility was developed as a research guidance tool to generate material balances, utilities consumptions, and capital cost estimates for the complex. This model was developed on a modular basis so that alternate and/or new processing options could be easily studied and evaluated. Since this model is PC based, entire plant sections (such as the naphtha and gas oil hydrotreaters, gas plant, and hydrogen production facilities) were represented by simplified Fortran input/output modules to minimize computer requirements and allow easy modification or expansion as new technologies become available.

In addition to modeling the entire complex for the baseline design and the improved baseline design case, the original baseline design case was modeled with all seven options. The improved baseline design case was modeled with option 6 only. These ASPEN/SP process simulation models can be extended to study selected combinations of the above options with both the original baseline design and the improved baseline design cases.

A separate LOTUS spreadsheet economics model was developed for use by the Pittsburgh Energy Technology Center to evaluate liquefaction economics and study various economic scenarios. This spreadsheet model will read a file generated by the ASPEN/SP process simulation model so that model results easily can be evaluated. The economics model was developed a separate spreadsheet model at PETC's request to provide maximum flexibility and allow rapid evaluation of numerous alternate scenarios using common software and minimal computer facilities.

The final model developed is a kinetic coal liquefaction reactor simulation using ASPEN/SP software. This two-reactor model considers the effects of vapor/liquid equilibrium and bed hydrodynamics in predicting reactor performance. It was designed to study the effects of the various flow and catalyst parameters on reactor sizing. This model was not integrated into the entire coal liquefaction complex simulation model to keep the model simple, fast and easy to use. This model, however, can be used iteratively with the ASPEN/SP simulation model of the entire complex to study how reactor behavior influences the entire complex.

12. Conclusions

- Models developed in this study are valuable research guidance tools to evaluate future advancements in coal liquefaction technology.

- The results of the economics evaluation showed that the current direct coal liquefaction technology ultimately (for a very optimistic scenario) may produce coal liquids in a grassroots plant that are competitive with crude oil priced at about 31.00 $/bbl. Products from initial plants, however, will be more costly because of the requirement of more spare trains, equipment, and resulting higher engineering and construction costs.

- Further cost reductions must come from schemes that reduce capital costs (e.g., slurry reactors or close-coupled hydrotreaters), reduce feedstock costs (e.g., low rank coals), integration with existing oil refineries, or locations at sites which offer feedstock and/or construction cost advantages.

13. Recommendations

Over the past decade or so, significant improvements have resulted in the reduction of the cost of direct liquefaction of coal. However, further advancement is necessary to make the process more economical. Sensitivity analysis on economics suggests that both capital costs and raw material costs have a significant impact on the economics of direct coal liquefaction.

Some areas worth considering for future economics studies include:

- Lower Rank Feed Coal

  The use of lower rank coals rather than the Illinois No. 6 bituminous coal used in this study can reduce coal costs by over 50%. A contract extension has just been approved by DOE to study the economics of direct liquefaction of a lower rank coal at a Wyoming location.

- Effect of Coal Cleaning on Coal Conversion

  The effect of coal cleaning on coal reactivity and conversion warrants future study. In the absence of experimental data, this study assumed that the degree of coal cleaning had no effect on its reactivity. If deeper coal cleaning removes material that is less reactive, then it could produce some additional benefits.

- Other Types of Reactor Designs

  The use of reactor designs such as slurry reactors with dispersed and/or soluble catalysts is an important area of future study. The operating trains having only slurry reactors are expected to be less expensive than the ebulated bed reactors.

- Different Plant Location

  Consideration should be given on a different plant location other than the southern Illinois mine mouth location used in this study. Although the plant construction costs along the gulf coast are less expensive than those in the midwest, the reduction, however, may be offset by increased coal and refuse transportation costs. The selection of a strategic location may provide the utilization of a variety of feed coal and enhance product marketing flexibility.

- Close-coupled Upgrading of Coal Liquids

  Investigation of close-coupled liquefaction and upgrading of the coal liquids rather than the conventional separation followed by hydrotreating steps used in this study is another recommended area for future study. Capital costs should be reduced by close-coupled upgrading in which most of the coal liquefaction reactor products are immediately mixed with additional hydrogen and passed over a hydrotreating catalyst before being cooled, depressurized and separated. However, at this time, insufficient information is available for designing a plant utilizing this concept.

- Developing a coal liquids product quality data reference library.

  This lack of data was identified both during the process design and when estimating the value of the liquefaction products. The availability of accurate physical property data will allow lower cost plant designs and allow definitive assessments of the economics of coal liquefaction by reducing the uncertainties associated with the product evaluation.

In addition, there is a continued need to carry on the basic research to reduce the liquefaction pressure and to develop improved liquefaction catalysts.

Another area of importance for future investigations relates to some degree of environmental concern of utilizing coal liquids as transportation fuels. This needs to be addressed in terms of the pending regulations based on the 1990 amendments of the Clean Air Act.

CALCULATION SHEET

BECHTEL

P.O. BOX 2166
HOUSTON, TEXAS 77252-2166

CALC. NO. ________

SIGNATURE ________ DATE ________ CHECKED ________ DATE ________

PROJECT ________ JOB NO. ________

SUBJECT ________ SHEET ________ OF ________ SHEETS ________

16,503 TPD MAF TO LIQUIFER

$$\frac{16{,}503}{18641} = \frac{X}{(18641+7403)} = \frac{X}{26044}$$

X = 23057 TPD TO GASIF & LIQ (MAF)

$$X = 23057/1.102 = 20922.8675 \text{ TPD METRIC}$$

$$80996 \text{ BPD}/20922.8 = 3.87$$

COAL TO LIQ ONLY

$$\frac{80996 \times 1.102}{16503} = 5.4$$

WITH GAS FOR H2

$$\frac{1718.9 \times 10^3 \text{ Lbs/HR MAF} \times 24}{2000} = 20{,}626.8 \text{ TPD}$$

$$\times \frac{1}{1.102} = 18717.6 \text{ MTPD}$$

$$\frac{80996}{18717.6} = 4.32$$

TRANSMISSION VERIFICATION REPORT

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NAME : T*D MGNT GROUP
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DATE,TIME	03/19 07:49
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DURATION	00:01:40
PAGE(S)	05
RESULT	OK
MODE	STANDARD ECM

FAX

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Date March 19, 2003

Number of pages including cover sheet ____

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REMARKS:

☐ Urgent ☒ For your review ☐ Reply ASAP ☐ Please comment

Eric

Evidently, the coal feed rates in the table within the Summary Report seem to be Wrong! Attached are the mass balance sheets for the Baseline and Improved Baseline cases. In addition, it appears that the cases used two different coals. Their properties are attached also. I don't have the heating values of the coals. You can calculate them from the properties.

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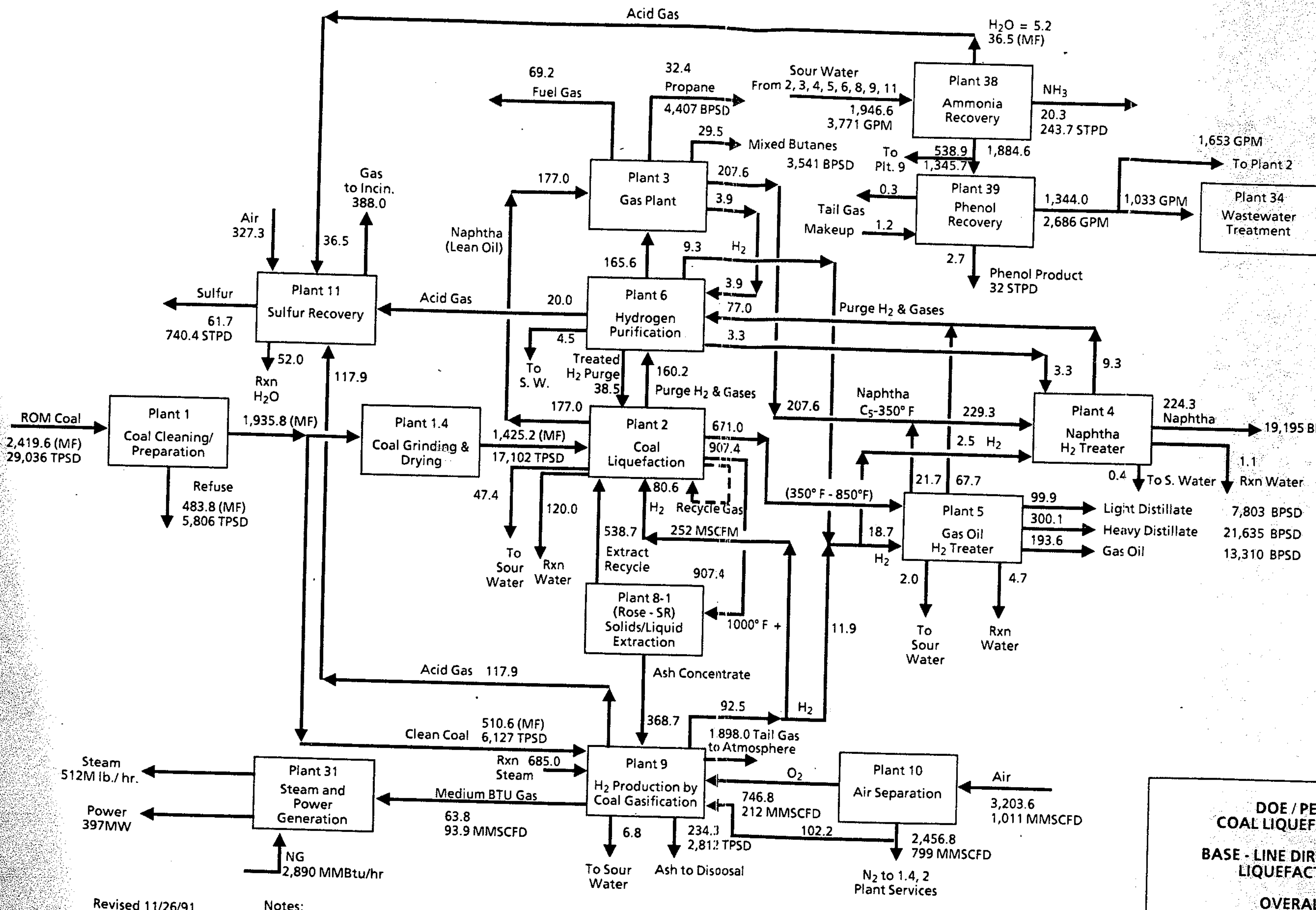
If you need anything more, please let me know.

Sheldon J. Kramer



DOE / PETC
COAL LIQUEFACTION

BASE - LINE DIRECT COAL LIQUEFACTION

OVERALL MATERIAL BALANCE

Figure 5.1

Notes:

1. Flow rates are in MLB/HR unless noted and on dry basis
2. Simplied water flow distribution diagram is shown on Figure 41.1
3. Minor streams including steam, water, sour water, and make-up amine are not shown on this diagram
4. Flow rates around plants #38, 39, 34 are shown on wet basis