1 of 1

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THE ECONOMICAL PRODUCTION OF
ALCOHOL FUELS FROM
COAL-DERIVED SYNTHESIS GAS

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EXECUTIVE SUMMARY

In Task 1, catalyst preparation is actively proceeding at both WVU and UCC&P. Molybdenum based catalyst materials are now being produced at WVU. The work at Union Carbide on transition metal oxide supported catalysts has focused on the lanthanide oxides. The radioactive properties of the actinide oxides make them impractical to study in light of current government regulations.

The reaction modeling for alcohol synthesis has completed phase 1 and is being tested on literature data.

Catalyst testing equipment is ready to run at UCC&P. Reactor construction at WVU is anticipated to be complete by the end of summer 1993.

In Task 2, four base cases have been completed. Base Cases 1 and 2 employ a Texaco gasifier. In Base Case 1, steam reforming of natural gas is used to increase the $H_2:CO$ ratio of the syngas to the required value of 1.2. In Base Case 4, a sour gas shift converter is used to increase the $H_2:CO$ ratio. The estimated capital investment for both of these processes is \$560 MM, and they provide identical pay back periods as a function of selling price of the alcohol fuel product. Base Case 2 employs a Lurgi gasifier. This case was investigated in order to determine whether the sale of coal by-products makes the economics more favorable. Under the assumption that all by-products can be sold, the capital investment for this process is \$930 MM, and the pay back period is higher than for the Texaco cases. Since it is unlikely that all by-products can be sold, this process will not be pursued any further. A base case has also been prepared in which natural gas is the source of syngas. This case, Base Case 3, is for comparison purposes only. The capital investment for this process is only \$212 MM, and the pay back period is 1 years less than for Base Cases 1 and 4.

Since the last report, these base cases have been altered to reflect a more realistic product distribution in the alcohol synthesis reactor. The formation of excess carbon dioxide plus small amounts of

methane, ethane, and esters in the reactor has been included in the analysis. Due to the conversion of carbon into these undesirable products, more coal and larger equipment is required to make the same amount of product. This is why costs have increased from previous reports. The separation sequence subsequent to the reactor has not yet been studied in detail since an exact product composition is not yet known. This will be studied in the future.

The optimization technique known as simulated annealing is being extended for use in optimizing the coal to syngas to higher alcohols process. Previously, this novel optimization technique has only been applied to specialized problems such as heat exchanger integration, batch process scheduling, and separation sequence synthesis. The latter application will be implemented in this process. However, since simulated annealing is most powerful for optimization of processes involving discrete choices, there is a more important application to this process. In the synthesis of syngas, there are several blocks which involve discrete choices, such as the gasifier and acid gas clean up. Techniques are under development which will allow optimization of the syngas production portion of the process.

Preliminary economic investigations have focused on cost reduction measures in the production of syngas from coal. A spread sheet model has been developed which can determine the cost of syngas production based upon the cost of equipment and raw materials and the market value of energy and by-products. In comparison to natural gas derived syngas, coal derived syngas is much more expensive, suggesting a questionable economic status of coal derived alcohol fuels. While it is possible that use of less expensive coal or significant integration of alcohol production and electricity production may reduce the cost of coal derived syngas, it is unlikely to be less costly to produce than syngas from natural gas.

Fuels evaluation is being conducted in three parts. First, standard ASTM tests are being used to analyze the blend characteristics of higher alcohols. Second, the performance characteristics of higher alcohols are being evaluated in a single-cylinder research engine. Third, the emissions characteristics of higher alcohols are being investigated. The equipment is still under construction and the measurement techniques are still being developed. Of particular interest is n-butanol, since the MoS_2 catalyst produces only linear higher alcohols. There is almost no information on the combustion and emission characteristics of n-butanol, hence the importance of gathering this information in this research.

TASK 1. REACTION STUDIES

1.1 Introduction

The objective of Task 1 is to prepare and evaluate catalysts and to develop efficient reactor systems for the selective conversion of hydrogen-lean synthesis gas to alcohol fuel extenders and octane enhancers.

Task 1 is subdivided into three subtasks: 1.1 laboratory and equipment setup; 1.2 catalysis research; and 1.3 reaction engineering. Research at West Virginia University is focused on molybdenum based catalysts. Parallel research being done at Union Carbide in South Charleston, WV is focused on lanthanide oxide supported catalysts.

1.2 Accomplishments, Results and Discussion

1.2.1 Laboratory Setup

Parts and equipment for the reactor systems are being collected prior to reactor construction this summer. Details on the unit design plans were provided in Quarterly Technical Progress Report 5, January, 1993.

1.2.2 Molybdenum Based Catalyst Research

Molybdenum catalyst preparations at WVU are being investigated using four approaches:

- 1). Synthesis and thermal decomposition of heterometallic inorganic and organometallic sulfide compounds.
- 2). Synthesis of supported and unsupported Chevrel phase compounds ($M'Mo_6S_8$) through the use of water soluble and refractory precursors.
- 3). Elevated temperature vapor phase synthesis of mixed metal sulfides and/or nitrides by the reaction of volatile metal carbonyls and halides with reactive gases.
- 4). Synthesis of molybdenum nitrido compounds by thermal and photolytic decomposition of a molecular molybdenum azide compound ("MoNN₃Py").

Approach 1

Based on a literature review, the following organometallic compounds have been selected for evaluation: $Cp^*_2Mo_2Fe_2(CO)_8$, $Cp_2Mo_2Co_2S_3(CO)_4$, $Cp_2Mo_2Ni_2S_4(CO)_2$, $Cp_2Mo_2Co_2S_4(CO)_2$, $Cp_2Mo_2Fe_2S_4(CO)_6$, $(NEt_4)_2\{M(SPh)_4[Mo(CO)_4]_2$ ($M=Ni, Co$) ($Cp=C_5H_5$), $Cp^*=(C_5Me_5)$. The compounds will be prepared and decomposed thermally in H_2S , vacuo and inert-gas

environments to produce intimately mixed metal sulfide catalysts. The starting materials are being purchased or synthesized. An undergraduate chemistry major has been hired for the summer to work specifically on the synthesis of these organometallic compounds.

Approach 2

The water-soluble Chevrel-phase precursor $(\text{NH}_4)_2\text{Mo}_3\text{S}_{13}$ has been prepared by adding 120 ml of a polysulfide solution (prepared by bubbling H_2S through a suspension of 27 g of S_8 in 150 ml of 10% $\text{NH}_3(\text{aq})$) to 20 ml of an ammonium molybdate solution (prepared by dissolving 4.0 g of $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$ in 20 ml of water) and heating for 5 days at 95 °C. $(\text{NH}_4)_2\text{Mo}_3\text{S}_{13}$ was characterized by X-ray single crystal and powder diffraction. The X-ray powder pattern matches a simulated pattern and the triangular disulfide bridged molybdenum cluster has been identified by single crystal X-ray studies. The potassium analog $(\text{K}_2\text{Mo}_3\text{S}_{13})$ has also been made by a similar procedure where a potassium polysulfide solution was used instead of the ammonia solution. $(\text{NH}_4)_2\text{MoS}_4$ has been obtained for use in the preparation of supported Chevrel phase compounds.

Approach 3

The starting materials, $\text{Mo}(\text{CO})_6$ and $\text{Co}_2(\text{CO})_8$ have been obtained and sublimed for use. $\text{Fe}(\text{CO})_5$, NbCl_5 , TaCl_5 , ZrCl_4 , HfCl_4 will also be used when the reactor system is fully tested. A Lindberg single zone 27" long furnace with ramp/setpoint controller has been purchased and wired in the lab. A second Lindberg furnace has been modified for use in smaller reactions and a Omega temperature control unit has been built by the chemistry staff for use with the small furnace. A quartz reactor has been designed and constructed by the departmental glassblower (see Figure 1.1). The reactor is comprised of two concentric quartz tubes which are separated by 4 mm. The volatile metal compounds will be heated and carried by a helium gas stream into the heating zone of the furnace. The reaction with the reactive gas (H_2S or NH_3) will occur three inches from the furnace center and will be facilitated by the reactive gas entering the inner tube from eight opposing holes in the inner quartz tube. The metal stoichiometry of the catalysts produced from this technique will depend on the vapor pressure of the metal compound and therefore can be varied in a continuous manner by variation of the sublimation temperature. A vacuum line is being rebuilt for use with the reactor and a purification column for removal of oxygen and water is being set up for the Helium carrier gas.

Figure 1.1 Diagram of a quartz reactor comprised of two concentric quartz tubes (56 mm and 48 mm) for reaction of volatile metal compounds with reactive gases, specifically H₂S. The volatile metal compounds (e.g., Mo(CO)₆ or Co₂(CO)₈) will be sublimed into the He carrier gas. H₂S will be introduced through the eight opposing holes in the inner tube where the sulfidation will occur at temperatures ranging from 500 °C to 1000 °C.

Approach 4

A molybdenum azide compound, which has been characterized by elemental analyses, IR and NMR has been synthesized by the following reactions in refluxing pyridine:

Thermal decomposition of "MoNN₃Py" occurs around 270 °C, depending on the conditions, and produces a material with a Mo:N ratio of 1:1.8. TGA/IR, DTA and mass spectral studies of the decomposition have been completed. N₂ comprises 90-95 % of the volatile decomposition products at 270 °C. Prior to the decomposition, pyridine was the primary product observed when heating. Because this material undergoes a gas-evolving molecular decomposition at 270 °C, a high surface area was predicted for this material. Surface area studies have been completed for MoNN₃Py decomposed at 280 °C in flowing ammonia and under vacuum (see Table 1.1). The surface areas of the decomposed products are extremely low for catalysts, which was the primary reason for using these materials. From the data it is probable that the ammonia causes annealing of the phase. The room temperature photolytic decomposition will be investigated, which should circumvent the apparent surface area reduction occurring at higher temperatures. The molybdenum nitrides produced from this decomposition will be evaluated for their catalytic ability as those measurements become available.

Table 1.1 N₂ Adsorption/Desorption Surface Area Studies of MoNN₃Py Decomposed in Ammonia and Under Vacuum at 280 °C

Decomposition Environment	Temperature (Final °C)	Time at Final Temperature	Surface Area (M ² /gram)	
			BET	T Plot*
Ammonia	280	4 hours	0.5	15.4
Vacuum	280	4 hours	1.5	24.0

*Meso and macropores only

BET surface areas are measurement standard. T-plot is a method of approximating large pore surface area. This generally agrees within 20% of BET value.

1.2.3 Lanthanide Oxide Supported Catalyst Research

Our initial focus was the synthesis and screening of lanthanide or actinide oxide supported transition metal catalysts. However, we recently discovered that the radioactivity of the actinides makes them impractical to use both in the lab and as commercial catalysts. Thus, we are changing the focus of our study somewhat to include only the lanthanides.

Following the leads developed at UCC in the early to mid 1980's, we were first going to examine copper on thorium promoted with alkali (3). We wanted to first synthesize the best catalyst found from that study and repeat the results of alcohol production from syn gas. We were ready to synthesize that material, but when we contacted our safety personnel to determine the proper handling and disposal of radioactive thorium, we discovered the disposal cost of even small amounts of thorium, although only slightly radioactive, would be prohibitive (at least \$7000 for grams of thorium). And, all equipment and other materials (catalyst testing equipment, alcohol products, catalyst preparation wastes and equipment) could be considered radioactive waste as well. Therefore, we decided to exclude all radioactive elements from the study.

1.2.4 Reaction Engineering

The three FORTRAN programs, PMBR1, CSTR1, and PFTR1, developed to simulate higher alcohol synthesis reactions conducted in perfectly mixed batch reactor (PMBR), continuous stirred-tank reactor (CSTR), and plug-flow tubular reactor (PFTR), have been modified to create their second version, PMBR2, CSTR2, and PFTR2, for execution on VAX. The first versions of the programs, developed for execution on IBM RISC/6000, were described in the previous quarterly report.

The three reactor models, which serve as the basis of the programs, are listed in Table 1.2. All six programs have been tested on a higher alcohol synthesis reaction scheme proposed by Tronconi et al. [IEC Res., 26, 2122 (1987)] which, as shown in Table 1.3, consists of 5 reactions and 8 components. They conducted their experiments in a tubular fixed-bed integral reactor packed with K₂O-promoted Zn-Cr oxide catalyst, and presented mole-fraction vs. space-time data. Our simulation results using PFTR1 and PFTR2 match their tubular-reactor experimental data well. Some typical results obtained using PMBR2, CSTR2, and PFTR2 are presented in Figures 1.2 to 1.9 mainly to illustrate the capabilities of these programs.

The computer programs for PFTR and CSTR were developed to simulate the two laboratory reactors (plug-flow reactor and recirculating autoclave reactor) being designed and constructed at WVU for the project. The computer program for PMBR can be used to simulate the autoclave reactor operated in batch mode. By replacing the rate expressions shown in Table 1.3 by power-law kinetics and comparing the simulation results with the experimental data for the catalysts being developed, the simulation programs can also be used to determine the apparent kinetics of the catalysts being developed. Since the parameters of the models and the programs can be easily changed to simulate a wide range of different operation conditions of the reactors, the programs also provide useful qualitative information about the behaviors of the reaction systems being investigated.

Table 1,2

Reactor Model

- **Perfectly Mixed Batch Reactor (PMBR)**

$$\frac{dN_j}{dt} = W \sum_{i=1}^{nr} v_{ij} r_i, N_j(0) = N_{j0}; j = 1, 2, \dots, nc.$$

- **Continuous Stirred-Tank Reactor (CSTR)**

$$\frac{dN_j}{dt} = F_{j0} - F_j + W \sum_{i=1}^{nr} v_{ij} r_i, N_j(0) = N_{j0}; j = 1, 2, \dots, nc.$$

- **Plug-Flow Tubular Reactor (PFTR)**

$$\frac{dF_j}{dW} = \sum_{i=1}^{nr} v_{ij} r_i; F_j(0) = F_{j0}; j = 1, 2, \dots, nc.$$

where

N_j : moles of component j at any time

N_{j0} : moles of component j present initially

F_j : molar flow rate of component j in CSTR or PFTR

F_{j0} : molar flow rate of component j in feed

v_{ij} : stoichiometric coefficient for component j in the i th reaction

r_i : rate of reaction in reaction i

W : weight of catalyst

nr : number of reactions

nc : number of components

t : reaction time (CSTR or PMBR)

Table 1.3

Lumped Kinetics for Higher Alcohol Synthesis *

- Reaction Scheme :

where

N_c = carbon number averaged over all higher oxygenated products

HA = a pseudo component representing higher (C_2 - C_8) alcohols

OL = a pseudo component representing olefin and C_{2+} hydrocarbons

- Rate Expressions :

$$\begin{aligned} r_1 &= k_1 \left[P_{\text{CO}}^2 P_{\text{H}_2} - \frac{P_{\text{CH}_3\text{OH}}}{K_1} \right] ; & r_4 &= k_4 P_{\text{H}_2} \\ r_2 &= \frac{k_2 P_{\text{CH}_3\text{OH}}}{\left[1 + K_w P_{\text{H}_2\text{O}} \right]} ; & r_5 &= k_5 \left[P_{\text{HA}} \right]^{\frac{1}{2}} \\ r_3 &= k_3 \left[P_{\text{CO}} P_{\text{H}_2\text{O}} - \frac{P_{\text{CO}_2} P_{\text{H}_2}}{K_3} \right] \end{aligned}$$

Where

k_i = rate constant

K_i = equilibrium constant or kinetic parameter

* Tronconi et al. (1987), K_2O -Promoted Zn - Cr Oxide Catalyst

Figure 1.2
PERFECTLY MIXED BATCH REACTOR (PMBR)

Figure 1.3
PLUG-FLOW TUBULAR REACTOR (PFTR)

Figure 1.4

CONTINUOUS STIRRED-TANK REACTOR (CSTR)

Figure 1.5
CONTINUOUS STIRRED-TANK REACTOR (CSTR)

Figure 1.6

PERFECTLY-MIXED BATCH REACTOR (PMBR)

Figure 1.7

PLUG-FLOW TUBULAR REACTOR (PFTR)

Figure 1.8

CONTINUOUS STIRRED-TANK REACTOR (CSTR)

Figure 1.9
CONTINUOUS STIRRED-TANK REACTOR (CSTR)

1.3 Conclusions and Recommendations

1.4 Future Plans

Reactor construction at WVU is anticipated to be complete by the end of summer 1993.

The decision to exclude all radioactive elements from this study has delayed the start of catalyst synthesis at Union Carbide. Catalyst development at UC will proceed with the contract using only the lanthanides. Since the lanthanides and actinides are similar, we shouldn't be hurting our efforts. Also, since thorium is fairly basic, we will first replace thorium in the catalyst prep from our earlier study (1) with a basic lanthanide like cerium. In fact, the earlier study included some materials using cerium and we can use those results for comparison.

Thus, we will start by preparing a material with the composition $\text{Cu}_{0.63} \text{Ce}_{0.18} \text{Zr}_{0.09} \text{K}_{0.1}$ and then test that catalyst in the production of fuel alcohols from syn gas and compare the results with the results from our previous study. In the near future, other catalysts will have similar compositions with different lanthanides replacing cerium as we explore the roles of the catalyst components on catalyst performance.

US Patent 4,943,551 (Union Carbide Corporation)

1.5 APPENDICES

1.6 References for Task 1

1. The Economical Production of Alcohol Fuels from Coal Derived Synthesis Gas, DOE Contract No. DE-AC22-91PC91034, Quarterly Technical Progress Report 5, Reporting period October 1, 1992 through December 31, 1992.
2. Tronconi, IEC Research, v26, p2122, 1987.
3. US Patent 4,943,551, Union Carbide Corporation.
4. Rase, Howard F., *Chemical Reactor Design for Process Plants, Volume 2*, John Wiley & Sons, New York, 1977, pp.133-138.

TASK 2. PROCESS SYNTHESIS AND FUEL EVALUATION.

2.1 Introduction

The objective of Task 2 is to use process synthesis and fuel evaluation studies to optimize the overall conversion process from choice of raw material feedstocks to final product slate.

2.2 Accomplishments, Results and Discussion

2.2.1 Process Design

There are four base case designs which have been developed. The purpose of developing this many base cases is to have a set of designs with different major features in order to determine which major features are most economical. The base cases are as follows:

1. Texaco gasifier with steam reforming of natural gas
2. Lurgi gasifier
3. Natural gas only (for comparison purposes only)
4. Texaco gasifier with sour gas shift converter

Additional base cases with the Shell gasifier system will also be developed as soon as economic and material balance data are available.

All of the base cases produce syngas at the same temperature and pressure and with the same $H_2:CO$ ratio. The alcohol synthesis loop, which has not yet been studied in detail, is identical for all of the base cases. A change has been made since the last quarterly report to include CO_2 , light hydrocarbons and esters which are formed in the reactor. The material balances and economics have been adjusted to account for these changes. As a result, capital costs have increased since more carbon is being converted to unwanted products, requiring more coal and larger equipment to produce syngas.

In the following sections, the equipment and economics for each base case are discussed and a spread sheet containing material and energy balances for each case is included.

Important information concerning decisions which were made for the creation of the base cases is contained in Quarterly Technical Progress Report 5, January, 1993.

2.2.2 Base Case 1

Appendix 2.1 contains a brief description of each of the units in the block flow diagram, Figure 2.1. All capital cost data in this report, except where otherwise specified, has been estimated from similar installations described in the Houston Area Medium-BTU Coal Gasification Project Final Report, published in June 1982 by Union

Carbide (All references to material in this report will be referred to as Houston). A factor of 0.65 was used for all exponential scaling, with the base case approximately 0.25 times the size of the facility described in the Union Carbide report. The plant consumes 1.0 million metric tons of coal, 1.2 million metric tons of oxygen, 0.13 billion standard cubic meters of natural gas, and produces 0.5 million metric tons of mixed alcohols per year.

2.2.2.1 Stand Alone Compressors and Power Summary for Base Case 1

There are 5 compressors which are not included in any of the blocks. Their inlet, outlet, pressure change, power rating, and installed capital cost are listed below. Following that is a summary of the total plant power output/input.

FUNCTION	INLET STREAM	P (kPa)	OUTLET STREAM	P (kPa)	POWER (MW)	COST (MM\$)
Air Prep	-	100	1	500	-25.3	0.7
O ₂ Prep	2	100	9	8000	-7.9	13.7
Reform Comp	17C	200	17	8000	-12.4	14.8
Rxtr Prep	22	8000	26	14000	-5.2	9.7
Recy Comp	56A	12500	56B	14000	-0.7	2.0
Total compressor needs					-51.5	
Other in plant needs					-8.2	
Total produced in steam and gas turbines					96.0	
Net power output					36.3	
Total installed compressor costs (1992 dollars)						40.4

2.2.2.2 Total Estimated Capital Investment (MM\$) for Base Case 1

Synthesis Gas via Methane	16.8
Coal Preparation	47.7
Texaco Gasifier	163.7
Slag Handling	3.0
Steam/Power Generation	89.3
Synthesis Gas Heat Recovery	7.8
Cryogenic Oxygen Production	76.7
Rectisol(Acid Gas Separation)	38.2
COS Hydrolysis	
Claus (Sulfur Recovery)	11.1
Beavon	4.2
MoS ₂ Alcohol Synthesis Loop	40.0
CO ₂ Removal in Alcohol	
Synthesis Loop	15.6
Other Compressors	40.9

TOTAL 555.0

2.2.2.3 Overall Economic Evaluation for Base Case 1

The following table gives the totals and breakdowns for the yearly operating costs as well as the total installed cost for the plant.

TOTAL ESTIMATED INSTALLED CAPITAL COST (MM\$)	555.0
TOTAL ESTIMATED OPERATING COSTS (MM\$/YR)	85.0
Coal (\$33/metric ton delivered)	26.6
Natural Gas (\$85/m ³)	13.3
Other Expenses	45.1
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS) (MM\$/YR)	22.2
Power (\$0.05/kW-hr)	14.7
Slag (\$5.5/metric ton) (6)	0.5
Sulfur (\$300/metric ton) (7)	7.0

Credits for nitrogen, argon, and other rare gases have not been included because prices were not available and potential markets have not yet been identified.

BASE CASE #1

Rev 1 7/2/92 Rev 2 8/5/92 Rev 3 8/19/92 Rev 4 12/7/92 Rev 5 3/26/93

FIG. CHART FOR BASE CASE : - FIGURE 2.1

Base Case 1	001	001A	002	003	004	006	008	009	010	011
Ar	118.2	118.2	0.0	0.0	0.0	118.2	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5618.7	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	C.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	4105.2	0.0	0.0	0.0
CO2	4.1	4.1	0.0	0.0	0.0	0.0	1483.4	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	3.5	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4.6
H2	0.0	0.0	0.0	0.0	0.0	0.0	3026.7	0.0	2296.0	0.0
H2O	305.5	305.5	0.0	0.0	0.0	0.0	3893.0	0.0	64.7	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	71.9	0.0	0.0	0.0
N2	9898.3	9898.3	0.0	9898.3	7161.4	0.0	45.6	0.0	49.7	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	8.3	0.0	0.0	0.0
O2	2661.1	2661.1	2661.1	0.0	0.0	0.0	0.0	2661.1	442.5	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	75.5	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	105.2	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	26.6	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	12987.2	12987.2	2661.1	9898.3	7161.4	118.2	12637.6	2661.1	8652.3	4.6
kg/hr	372715.0	372715.0	85155.2	277152.4	200519.2	4728.0	260630.7	85155.2	101879.0	460.0
Temp. (C)	262.0	25.0	25.0	25.0	25.0	25.0	1300.0	40.0	25.0	25.0
Press. (KPA)	517.1	103.4	517.1	517.1	517.1	517.1	8135.8	8135.8	103.4	103.4

• FLOW TABLE FOR BASE CASE 1 - TABLE 2.1

	012	013	014	015	017	017A	017B	17C	018	019
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	5618.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	567.3	0.0	567.4	0.0	4105.2	0.0
CO2	0.0	0.0	0.0	0.0	132.4	0.0	132.8	0.0	1483.4	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.5	0.0
CaCO3	0.0	4.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	2296.0	0.0	0.0	2233.2	0.0	2233.3	0.0	3026.7	0.0
H2O	4696.7	4761.4	0.0	1656.0	6.6	3899.6	823.1	776.5	3893.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	72.0	0.0
N2	0.0	49.7	0.0	0.0	0.0	0.0	0.0	0.0	45.6	2736.9
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.3	0.0
O2	0.0	442.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	75.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	105.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	700.7	0.0	4.8	0.0	0.5	0.0	26.6	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	4696.7	13353.6	0.0	1656.0	2939.5	3899.6	3756.6	776.5	12637.7	2736.9
kg/hr	84540.6	186879.6	11211.2	29808.0	26372.2	70192.8	41020.8	13977.0	262634.1	76633.2
Temp. (C)	25.0	25.0	135.0	300.0	25.0	25.0	926.9	25.0	25.0	25.0
Press. (KPa)	103.4	8135.8	200.0	200.0	8106.0	8106.0	202.0	202.0	8135.8	517.1

TABLE 2.1 (CONTINUED)

	020	022	022A	023	024	025	026	026A	027	028
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	18.0	0.0	0.0	0.0	0.0	18.0	0.0	622.5	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	649.4	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	143.7	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	36.2	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0	0.0	0.0
CO	0.0	4672.5	4625.8	0.0	0.0	0.0	4625.8	6937.6	0.0	0.0
CO2	0.0	0.0	0.0	969.5	565.5	80.7	0.0	1480.0	0.0	4.1
COS	0.0	0.0	0.0	0.0	0.0	3.5	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	5260.0	5207.3	0.0	0.0	0.0	5207.4	8332.7	0.0	0.0
H2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	138.8	0.0	305.5
H2S	0.0	0.0	0.0	0.0	0.0	72.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	2782.5	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	8.3	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.9	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.8	0.0	0.0
CH4	0.0	27.2	26.9	0.0	0.0	0.0	26.9	464.0	464.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.3	17.3	0.0
kmol/hr	18.0	9932.5	9833.1	969.5	3348.0	182.5	9833.2	18385.6	0.0	309.6
kg/hr	576.0	141785.2	140367.4	42658.0	102792.0	6715.9	140368.2	351255.8	7943.0	5679.4
Temp.(C)	25.0	25.0	25.0	25.0	25.0	25.0	310.0	310.0	50.0	25.0
Press.(KPA)	103.4	8106.0	8106.0	8106.0	8106.0	8106.0	14000.0	12666.0	12666.0	517.1

TABLE 2.1 - CONTINUED

	033	034	036	037	038	039	041	042	045	046
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	18.0	0.0	18.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	46.7	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	78.8	0.0	80.7	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	4.6	0.0	0.0	4.6	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	52.6	0.0	0.0	0.0	0.0	0.0
H2O	0.0	252.2	252.2	0.0	0.0	0.0	0.0	0.0	64.7	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	60.1	0.0	10.6	0.0
N2	0.0	0.0	0.0	0.0	0.0	99.2	0.0	112.0	112.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	6.6	0.0	8.3	0.0
O2	0.0	0.0	0.0	0.0	0.0	32.0	0.0	40.2	7.9	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	64.8
Al2O3	105.2	0.0	0.0	105.2	0.0	0.0	0.0	0.0	0.0	0.0
CaH2O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaH2O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0
Acetic acid	109.8	251.2	251.2	109.8	99.3	121.2	163.5	152.2	302.2	64.8
Acetic acid	1190.4	4521.6	4521.6	1190.4	1426.0	3920.4	6198.8	4422.4	9181.7	2073.6
Acetic acid	100.0	15.0	156.0	156.0	25.0	25.0	25.0	25.0	370.0	370.0
Acetic acid	5135.8	3447.4	3000.0	103.4	8106.0	15.0	15.0	103.4	103.4	103.4

TABLE 2.1 CONTINUED

	047	048	050	051	054	056	056A	056B	057	059
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	18.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	6937.6	6937.6	6937.6	0.0	6937.6
CO2	0.0	0.0	80.8	0.0	0.0	1480.0	0.0	0.0	1480.0	1480.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	20.0	0.0	0.0	0.0	8329.5	8329.5	8329.5	0.0	8329.5
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	16.1	0.0	128.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	6.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	4.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	7.2	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	484.3
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.3
kmol/hr	20.4	20.0	235.2	7.2	72.0	16747.1	15267.1	15267.1	1480.0	16747.1
kg/hr	588.4	360.0	7859.1	230.4	1296.0	276031.8	210911.8	210911.8	65120.0	283574.8
Temp. (C)	25.0	25.0	370.0	25.0	370.0	310.0	310.0	310.0	25.0	310.0
Press. (KPA)	103.4	15.0	103.4	103.4	103.4	12666.0	12666.0	14185.0	12666.0	12666.0

TABLE 2.1 - CONTINUED

[illegible]

2.2.3 Base Case 2

Appendix 2.2 contains a brief description of each of the units in the block flow diagram, Figure 2.2. A factor of 0.65 was used for all exponential scaling. The plant consumes 2.4 million metric tons of coal, 1.4 million metric tons of oxygen, and produces 0.5 million metric tons of mixed alcohols per year.

2.2.3.1 Stand Alone Compressors and Power Summary for Base Case 2

There are 4 compressors which are not included in any of the blocks. Their inlet, outlet, pressure change, power rating, and installed capital cost are listed below. Following that is a summary of the total plant power output/input.

FUNCTION	INLET STREAM	P (kPa)	OUTLET STREAM	P (kPa)	POWER (MW)	COST (MM\$)
Air Prep	-	100	1	500	-52.3	1.2
O ₂ Prep	2	100	9	8000	-19.2	24.5
Rxtr Prep	22	8000	26	14000	-7.1	11.9
Recy Comp	56A	12500	56B	14000	-0.9	2.4
Total compressor needs					-79.5	
Other in plant needs					-13.0	
Total produced in steam and gas turbines					209.0	
Net power output					116.5	
Total installed compressor costs (1992 dollars)						40.0

2.2.3.2 Total Estimated Capital Investment (MM\$) for Base Case 2

Coal Preparation	91.9
Lurgi Gasifier	269.7
Slag Handling	5.9
Steam/Power Generation	166.7
Cryogenic Oxygen Production	139.9
Rectisol (Acid Gas Separation)	121.9
COS Hydrolysis	
Claus (Sulfur Recovery)	21.5
Beavon	8.1
MoS, Alcohol Synthesis Loop	40.0
CO, Removal in Alcohol Synthesis Loop	15.6
Other Compressors	40.0
Pressure Swing Adsorption	10.0
TOTAL	931.2

2.2.3.3 Overall Economic Evaluation for Base Case 2

The following table gives the totals and breakdowns for the yearly operating costs as well as the total installed cost for the plant.

TOTAL ESTIMATED INSTALLED CAPITAL COST(MM\$)	931.2
TOTAL ESTIMATED OPERATING COSTS(MM\$/YR)	154.7
Coal (\$30/ton delivered)	73.0
Other Expenses	81.7
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS) (MM\$/YR)	146.6
Power (\$0.05/KW-hr)	47.3
Slag (\$5/ton) (5)	1.4
Sulfur (\$13.60/100 lbs.) (6)	18.9
Coal Tar/Liquid By-Products	79.0

Credits for purified nitrogen, argon, and hydrogen have not been included because prices were not available and no potential markets have been identified.

FIGURE 2.2 FLOW CHART FOR BASE CASE 2

Base Case 2	001	001A	002	003	004	006	008	009	010	011
Ar	205.1	205.1	0.0	0.0	0.0	205.1	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15580.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	4672.2	0.0	0.0	0.0
CO2	7.2	7.2	0.0	0.0	0.0	0.0	6395.1	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	8.4	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	14.3
H2	0.0	0.0	0.0	0.0	0.0	0.0	11123.0	0.0	6367.0	0.0
H2O	530.4	530.4	0.0	0.0	0.0	0.0	19618.0	0.0	179.3	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	200.8	0.0	0.0	0.0
N2	17180.0	17180.0	0.0	17180.0	7161.4	0.0	125.2	0.0	137.9	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	25.5	0.0	0.0	0.0
O2	4619.6	4619.6	4619.6	0.0	0.0	0.0	0.0	4619.6	1227.3	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	209.3	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	291.9	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	2382.8	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	22542.3	22542.3	4619.6	17180.0	7161.4	205.1	44551.0	4619.6	23992.7	14.3
kg/hr	646935.2	646935.2	147827.2	481040.0	200519.2	8204.0	836467.1	147827.2	282527.6	1430.0
Temp. (C)	262.0	25.0	25.0	25.0	25.0	25.0	1300.0	40.0	25.0	25.0
Press. (KPA)	517.1	103.4	517.1	517.1	517.1	517.1	8135.8	8135.8	103.4	103.4

TABLE 2.2 FLOW TABLE FOR BASE CASE 2

	G12	G13	G17A	G18	G19	G20	G22	G22A	G22AA	G23
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	15580.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	4672.2	0.0	0.0	4672.2	4625.5	4625.5	0.0
CO2	0.0	0.0	0.0	6395.2	0.0	0.0	0.0	0.0	0.0	383.2
COS	0.0	0.0	0.0	5.4	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	14.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	6367.0	0.0	1123.0	0.0	0.0	1123.0	11012.0	0.0	0.0
H2O	26840.0	27019.3	19618.0	19618.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	200.9	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	137.9	0.0	125.2	10019.0	0.0	0.0	0.0	5204.4	0.0
NH3	0.0	0.0	0.0	25.5	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	1227.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	209.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	291.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	2382.8	0.0	0.0	2382.8	2359.0	2359.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	26840.0	50847.0	19618.0	44551.1	10019.0	19.0	18178.0	17996.8	22188.3	3937.1
kg/hr	483120.0	767077.6	353124.0	836410.5	280532.0	376.0	191192.4	189282.0	322981.2	16832.4
Temp. (C)	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0
Press. (kPa)	103.4	8135.8	8106.0	8135.8	817.1	103.4	8106.0	8106.0	8106.0	8016.0

TABLE 2.2 (CONTINUED)

	024	025	026	026A	027	027A	028	033	034	036
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2121.4	0.0	0.0
CH3OH	0.0	18.0	0.0	622.5	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	649.3	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	143.7	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	36.2	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	4625.5	6937.2	0.0	0.0	0.0	0.0	0.0	0.0
CO2	2238.3	319.8	0.0	1479.9	0.0	0.0	7.2	0.0	0.0	0.0
COS	0.0	8.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	14.3	0.0	0.0
H2	0.0	0.0	5204.4	7812.9	0.0	5807.8	0.0	2278.3	0.0	0.0
H2O	0.0	0.0	0.0	138.7	0.0	0.0	530.4	0.0	272.5	272.5
H2S	0.0	200.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	10144.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	25.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1073.6	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	291.9	0.0	0.0
C3H6O2	0.0	0.0	0.0	17.9	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	11.8	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	2359.0	2796.1	2796.1	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	17.3	17.3	0.0	0.0	0.0	0.0	0.0
kmol/hr	12382.3	572.6	12188.9	20678.5	2813.4	5807.8	537.6	5779.5	272.5	272.5
kg/hr	382517.2	21911.3	177666.8	387507.8	45256.6	11615.6	9864.0	95572.4	4905.0	4905.0
Temp. (C)	25.0	25.0	310.0	310.0	50.0	25.0	25.0	1300.0	25.0	156.0
Press. (KPA)	8106.0	8106.0	14185.0	12666.0	12666.0	8106.0	517.1	8135.8	3447.4	103.4

TABLE 2.2 (CONTINUED)

	037	038	039	041	042	045	046	047	048	050
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	2121.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	18.0	0.0	18.0	0.0	0.0	0.0	18.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	46.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	341.2	0.0	319.8	0.0	0.0	0.0	319.8
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	14.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	2278.3	111.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	0.0	0.0	180.8	0.0	0.0	20.0	0.0
H2S	0.0	0.0	0.0	220.0	0.0	28.5	0.0	0.0	0.0	0.0
N2	0.0	0.0	89.2	0.0	346.4	346.4	0.0	49.7	0.0	396.1
NH3	0.0	0.0	0.0	18.7	0.0	25.5	0.0	0.0	0.0	25.5
O2	1073.6	0.0	32.0	0.0	124.3	33.9	0.0	13.2	0.0	37.1
S	0.0	0.0	0.0	0.0	0.0	0.0	180.8	0.0	0.0	0.0
Al2O3	291.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	23.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	5779.5	181.7	121.2	597.9	470.7	952.9	180.8	62.9	20.0	796.5
kg/hr	95572.4	1910.8	3520.4	23386.7	13676.8	30088.1	5785.6	1814.0	360.0	27358.7
Temp. (C)	156.0	25.0	25.0	25.0	25.0	370.0	370.0	25.0	25.0	370.0
Press. (KPA)	103.4	8106.0	103.4	103.4	103.4	103.4	103.4	103.4	103.4	103.4

TABLE 2.2 - (CONTINUED)

	051	054	056	056A	056B	057	059	063	064	065
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	622.5	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	649.3	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	143.7	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	36.2	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0	0.0
CO	0.0	0.0	6937.2	6937.2	6937.2	0.0	6937.2	0.0	0.0	0.0
CO2	0.0	0.0	1479.9	0.0	0.0	1479.9	1479.9	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	7812.3	7812.3	7812.3	0.0	7812.3	0.0	0.0	0.0
H2O	0.0	200.9	0.0	0.0	0.0	0.0	0.0	138.7	0.0	329.2
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	20.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.9	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.8	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	2796.1	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	17.3	0.0	0.0	0.0
kmol/hr	20.1	200.9	16229.4	14749.5	14749.5	1479.9	19042.8	168.4	1466.7	329.2
kg/hr	643.2	3616.2	274981.8	209866.2	209866.2	65115.6	320238.4	4859.6	62408.6	5925.6
Temp. (C)	25.0	370.0	310.0	310.0	310.0	25.0	310.0	25.0	25.0	25.0
Press. (KPA)	103.4	103.4	12666.0	12666.0	14185.0	12666.0	12666.0	12666.0	12666.0	103.4

TABLE 2.2 (CONTINUED)

	067	070	073	074	075
Ar	300.0	0.0	0.0	0.0	300.0
C	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	2830.7
COS	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	33000.0	33000.0	5973.4
H2S	0.0	0.0	0.0	0.0	0.0
N2	22000.0	0.0	0.0	0.0	22000.0
NH3	0.0	0.0	0.0	0.0	0.0
O2	6230.0	0.0	0.0	0.0	577.0
S	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0
CH4	0.0	2796.1	0.0	0.0	0.0
C2H6	0.0	17.3	0.0	0.0	0.0
kmol/hr	28530.0	2813.4	33000.0	33000.0	31681.1
kg/hr	827360.0	45256.6	594000.0	594000.0	878536.0
Temp. (C)	25.0	25.0	20.0	482.2	25.0
Press. (KPA)	103.4	101.3	10446.0	10446.0	101.3

TABLE 2.2 (CONTINUED)

2.2.4 Base Case 3

Appendix 2.3 contains a brief description of each of the units in the block flow diagram, Figure 2.3. A factor of 0.65 was used for all exponential scaling, with the base case approximately 0.25 times the size of the facility described in the Union Carbide report. The plant consumes 0.7 billion standard cubic meters of natural gas per year and produces 0.5 million metric tons of mixed alcohols per year.

2.2.4.1 Stand Alone Compressors and Power Summary for Base Case 3

There are two compressors which are not included in any of the blocks. Their inlet, outlet, pressure change, power rating, and installed capital cost are listed below. Following that is a summary of the total plant power output/input.

FUNCTION	INLET STREAM	P (kPa)	OUTLET STREAM	P (kPa)	POWER (MW)	COST (MM\$)
Rxtr Prep	22A	200	26	14000	-5.9	11.7
Recy Comp	56A	12500	56B	14000	-0.7	2.0
Total compressor needs					-6.6	
Other in plant needs					-6.6	
Total produced in steam and gas turbines					44.0	
Net power output					30.8	
Total installed compressor costs (1992 dollars)						13.7

2.2.4.2 Total Estimated Capital Investment (MM\$) for Base Case 3

Syngas Reforming	62.5
Rectison (Acid Gas Separation)	18.7
Pressure Swing Adsorption	10.0
MoS ₂ Alcohol Synthesis Loop	40.0
CO ₂ Removal in Alcohol Synthesis Loop	15.6
Steam/Power Generation	51.5
Other Compressors	13.7
TOTAL	212.0

2.2.4.3 Overall Economic Evaluation for Base Case 3

The following table gives the totals and breakdowns for the yearly operating costs as well as the total installed cost for the plant.

TOTAL ESTIMATED INSTALLED CAPITAL COST(MM\$)	212.0
TOTAL ESTIMATED OPERATING COSTS(MM\$/YR)	142.5
Natural Gas (\$85/m ³)	100.5
Other Expenses	42.0
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS) (MM\$/YR)	29.5
Power (\$0.05/kW-hr)	29.5

BASE CASE #3

FIGURE 2.3 FLOW CHART FOR BASE CASE 3

Base Case 3	014	015	017	017A	019	020	022	022AA	023
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H7OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C6H11OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	4625.5	0.0	0.0	0.0	4625.5	4625.5	0.0
CO2	0.0	0.0	670.3	0.0	0.0	0.0	0.0	0.0	432.2
CO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	16539.0	0.0	0.0	0.0	16539.0	5207.3	0.0
H2O	0.0	12520.0	6553.9	6553.9	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	720.6	0.0	0.0	0.0	0.0
N2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
A12O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	5295.9	0.0	0.1	0.0	0.0	0.0	0.1	0.1	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kmol/hr	5295.9	12520.0	28407.8	6553.9	720.6	18.0	21183.6	9832.9	402.2
Kg/hr	84734.4	225360.0	310094.2	117970.0	20176.8	576.0	162631.6	139930.2	17696.8
Temp. (C)	25.0	300.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0
Press. (kPa)	199.0	200.0	232.0	5106.0	207.0	103.4	8106.0	8106.0	8106.0

TABLE 2.3 FLOW TABLE FOR BASE CASE 3

	024	025	026A	027	028	036	056A	056B	057	058
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	622.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	0.0	649.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	0.0	143.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	0.0	36.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	0.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	4625.5	6937.3	0.0	0.0	6937.3	6937.3	6937.3	0.0	6937.3
CO2	234.6	0.0	1480.0	0.0	0.0	1475.6	0.0	0.0	1475.6	1475.6
CO5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	8207.3	8366.2	0.0	11350.0	8362.6	8362.6	8362.6	0.0	8362.6
H2O	0.0	0.0	138.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	720.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
A12O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	17.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	11.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.1	437.1	437.1	0.0	0.0	0.0	0.0	0.0	437.1
C2H6	0.0	0.0	17.3	17.3	0.0	0.0	0.0	0.0	0.0	17.3
kmol/hr	955.2	9632.9	18973.0	454.4	11350.0	16780.0	15300.1	15300.1	1479.9	17234.4
kg/hr	30499.2	139930.2	350877.6	7512.6	22700.0	276085.6	210970.0	210970.0	65115.6	293398.2
Temp. (C)	25.0	310.0	310.0	50.0	25.0	310.0	310.0	310.0	25.0	310.0
Press. (kPa)	8106.0	14165.0	12666.0	12666.0	8106.0	12666.0	12666.0	14185.0	12666.0	12666.0

TABLE 2.3 (CONTINUED)

	063	064	065	067	070	073	074	075
Ar	0.0	0.0	0.0	62.0	0.0	0.0	0.0	62.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	622.5	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	649.3	0.0	0.0	0.0	0.0	0.0	0.0
C3H7OH	0.0	143.7	0.0	0.0	0.0	0.0	0.0	0.0
C4H9OH	0.0	36.2	0.0	0.0	0.0	0.0	0.0	0.0
C5H11OH	0.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	471.8
CO5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	138.7	0.0	322.6	0.0	0.0	6200.0	6200.0	1249.8
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	4827.6	0.0	0.0	0.0	4827.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	1292.0	0.0	0.0	0.0	357.1
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O2	17.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	11.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	437.1	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	17.3	0.0	0.0	0.0
kmol/hr	168.4	1466.7	322.6	6181.6	454.4	6200.0	6200.0	6967.3
kg/hr	4859.6	62408.6	5806.8	178996.8	7512.6	111600.0	111600.0	192317.6
Temp. (C)	25.0	25.0	25.0	25.0	25.0	20.0	482.2	25.0
Press. (kPa)	11566.0	12666.0	103.4	103.4	101.3	10446.0	10446.0	101.3

TABLE 2.3 (CONTINUED)

2.2.5 Base Case 4

Appendix 2.4 contains a brief description of each of the units in the block flow diagram, Figure 2.4. A factor of 0.65 was used for all exponential scaling, with the base case approximately 0.25 times the size of the facility described in the Union Carbide report. The plant consumes 1.1 million metric tons of coal, 0.95 million metric tons of oxygen, and produces 0.5 million metric tons of mixed alcohols per year.

2.2.5.1 Stand Alone Compressors and Power Summary for Base Case 4

There are 4 compressors which are not included in any of the blocks. Their inlet, outlet, pressure change, power rating, and installed capital cost are listed below. Following that is a summary of the total plant power output/input.

FUNCTION	INLET STREAM	P (kPa)	OUTLET STREAM	P (kPa)	POWER (MW)	COST (MM\$)
Air Prep	-	100	1	500	-33.8	0.9
O ₂ Prep	2	100	9	8000	-12.4	18.4
Rxtr Prep	22	8000	26	14000	-5.2	9.7
Recy Comp	56A	12500	56B	14000	-0.7	2.0
Total compressor needs					-52.1	
Other in plant needs					-8.0	
Total produced in steam and gas turbines					86.0	
Net power output					25.9	
Total installed compressor costs (1992 dollars)					31.0	

2.2.5.2 Total Estimated Capital Investment (MM\$) for Base Case 4

Coal Preparation	51.8
Texaco Gasifier	188.1
Sour Gas Shift Converter	6.7
Slag Handling	3.3
Steam/Power Generation	83.1
Synthesis Gas Heat Recovery	8.4
Cryogenic Oxygen Production	82.6
Rectisol (Acid Gas Separation)	41.1
COS Hydrolysis	
Claus (Sulfur Recovery)	12.0
Beavon	4.5
Mos, Alcohol Synthesis Loop	40.0
CO, Removal in Alcohol	
Synthesis Loop	15.6
Other Compressors	31.0
TOTAL	568.2

2.2.5.3 Overall Economic Evaluation for Base Case 4

The following table gives the totals and breakdowns for the yearly operating costs as well as the total installed cost for the plant.

TOTAL ESTIMATED INSTALLED CAPITAL COST (MM\$)	568.2
TOTAL ESTIMATED OPERATING COSTS (MM\$/YR)	75.0
Coal (\$33/ metric ton delivered)	29.9
Other Expenses	45.1
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS) (MM\$/YR)	18.8
Power (\$0.05/kW-hr)	10.4
Slag (\$5.5/ metric ton) (5)	0.6
Sulfur (\$300/ metric ton) (6)	7.8

Credits for nitrogen, argon, and other rare gases has not been included because prices were not available and no potential markets have been identified.

BASE CASE # 4

FIGURE 2.4 FLOW CHART FOR BASE CASE 4

Base Case 1	CC1	CC1A	CC2	CC3	CC4	CC6	CC8	8a	CC9	CC0
Ar	154.5	154.5	0.0	0.0	0.0	154.5	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-324.7
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	5.8	5.8	0.0	0.0	0.0	0.0	5715.3	5715.3	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	2055.2	2055.2	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	4.9	4.9	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	4214.1	4214.1	0.0	3156.6
CO2	425.4	425.4	0.0	0.0	0.0	0.0	5420.0	5420.0	0.0	50.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	100.1	100.1	0.0	0.0
CO2	1370.0	1370.0	0.0	1370.0	7161.4	0.0	63.5	63.5	0.0	68.2
CO2	0.0	0.0	0.0	0.0	0.0	0.0	11.5	11.5	0.0	0.0
CO2	304.9	304.9	304.9	0.0	0.0	0.0	0.0	0.0	304.9	516.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	105.0
AL2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	146.6
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	37.2	37.2	0.0	0.0
CH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	1800.6	1800.6	3704.9	1370.0	7161.4	164.5	17631.9	17631.9	3704.9	12046.1
KG (H)	118559.2	118559.2	118556.8	395840.0	200519.2	6580.0	362861.5	362861.5	118556.8	118548.4
Temp. (C)	262.0	25.0	25.0	25.0	25.0	25.0	1300.0	25.0	40.0	25.0
Press. (KPa)	510.0	102.0	510.0	510.0	510.0	204.0	8030.0	8030.0	8030.0	102.0

Table 11 - Flow Table for Base Case 1

	011	012	013	017A	018	019	020	022	022A	023
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	7822.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H12O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	4672.7	0.0	0.0	4672.7	4625.9	0.0
CO2	0.0	0.0	0.0	0.0	3108.0	0.0	0.0	0.0	0.0	1864.8
COS	0.0	0.0	0.0	0.0	4.9	0.0	0.0	0.0	0.0	0.0
CaCO3	6.4	0.0	6.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	3196.6	0.0	5256.9	0.0	0.0	5256.9	5204.4	0.0
H2O	0.0	6539.0	6629.0	4377.2	4377.2	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	100.1	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	69.2	0.0	63.5	6618.6	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	11.5	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	616.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	105.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	146.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	37.0	0.0	0.0	37.1	36.7	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	6.4	6539.0	18591.5	4377.2	17631.8	6618.6	18.0	9966.7	9867.0	1864.8
kg/hr	640.0	117702.0	260190.4	78789.6	362859.9	185320.8	576.0	141943.0	140521.2	82051.2
Temp. (C)	25.0	25.0	25.0	25.0	300.0	25.0	25.0	25.0	25.0	25.0
Press. (KPa)	102.0	102.0	8030.0	8030.0	8030.0	510.0	102.0	8030.0	8030.0	102.0

TABLE 2.4 (CONTINUED)

	024	025	026	026A	027	028	033	034	036	037
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	18.0	0.0	622.6	0.0	0.0	0.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	649.4	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	143.7	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	36.2	0.0	0.0	0.0	0.0	0.0	0.0
C5H12O	0.0	0.0	0.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	4625.9	6937.9	0.0	0.0	0.0	0.0	0.0	0.0
CO2	1087.8	155.4	0.0	1480.1	0.0	5.8	0.0	0.0	0.0	0.0
COS	0.0	4.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	6.4	0.0	0.0	6.4
H2	0.0	0.0	5204.4	7806.4	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	138.8	0.0	425.4	0.0	349.7	349.7	0.0
H2S	0.0	100.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	6682.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	11.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	146.6	0.0	0.0	146.6
C3H8O2	0.0	0.0	0.0	17.9	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	11.8	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	36.7	473.8	473.8	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	17.3	17.3	0.0	0.0	0.0	0.0	0.0
kmol/hr	7769.9	289.9	9867.0	18350.9	491.1	431.2	153.0	349.7	349.7	153.0
kg/hr	234962.0	11012.5	140521.2	350376.0	8099.8	7912.4	15593.2	6294.6	6294.6	15593.2
Temp.(C)	25.0	25.0	310.0	310.0	50.0	25.0	1300.0	25.0	156.0	156.0
Press.(KPA)	102.0	102.0	14000.0	14000.0	14000.0	204.0	8030.0	3400.0	3400.0	102.0

TABLE 2.4 (CONTINUED)

	038	039	041	042	045	046	047	048	050	051
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	18.0	0.0	18.0	0.0	0.0	0.0	18.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5H12O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	46.7	0.0	46.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	155.4	0.0	155.4	0.0	0.0	0.0	155.4	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	52.6	0.0	52.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	0.0	90.1	0.0	0.0	20.0	0.0	0.0
H2S	0.0	0.0	105.0	0.0	10.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	20.0	20.0	156.0	156.0	0.0	22.3	0.0	178.3	0.0
NH3	0.0	0.0	11.5	0.0	11.5	0.0	0.0	0.0	11.5	0.0
O2	0.0	8.0	8.0	55.9	10.9	0.0	6.0	0.0	11.8	0.0
S	0.0	0.0	0.0	0.0	0.0	90.1	0.0	0.0	0.0	10.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.4	0.0	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	99.7	28.0	417.6	211.9	451.9	90.1	28.3	20.0	375.0	10.0
kg/hr	1419.2	816.0	13414.3	6156.8	14287.7	2883.2	816.4	360.0	12979.1	320.0
Temp. (C)	25.0	25.0	25.0	25.0	370.0	370.0	25.0	25.0	370.0	25.0
Press. (KPA)	8030.0	102.0	102.0	102.0	102.0	102.0	102.0	102.0	102.0	102.0

TABLE 2.4 (CONTINUED)

	054	056	056A	056B	057	059	063	064	065	067
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	52.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	622.6	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	649.4	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	143.7	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	36.2	0.0	0.0
C5H12O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0	0.0	0.0
CO	0.0	6937.9	6937.9	6937.9	0.0	6937.9	0.0	0.0	0.0	0.0
CO2	0.0	1480.1	0.0	0.0	1480.1	1480.1	0.0	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	7806.3	7806.3	7806.3	0.0	7806.3	0.0	0.0	0.0	0.0
H2O	100.1	0.0	0.0	0.0	0.0	0.0	138.8	0.0	422.5	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4827.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1242.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	17.9	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	11.8	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	100.1	16224.3	14744.2	14744.2	1480.1	16698.1	168.5	1466.9	422.5	6231.6
kg/hr	1801.8	274998.2	209873.8	209873.8	65124.4	282579.0	4861.4	62416.4	7605.0	177396.8
Temp. (C)	370.0	310.0	310.0	310.0	25.0	310.0	25.0	25.0	25.0	25.0
Press. (KPA)	102.0	12500.0	12500.0	14000.0	102.0	12500.0	102.0	102.0	102.0	102.0

TABLE 2.4 (CONTINUED)

	068	070	071	073	074	075
Ar	0.0	0.0	0.0	0.0	0.0	32.0
C	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0
C5H12O	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	508.5
COS	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0
H2O	10670.0	0.0	10670.0	3100.0	3100.0	948.3
H2S	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	0.0	4827.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	283.7
S	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	473.8	0.0	0.0	0.0	0.0
C2H6	0.0	17.3	0.0	0.0	0.0	0.0
kmol/hr	10670.0	491.1	10670.0	3100.0	3100.0	6600.1
kg/hr	192060.0	8099.8	192060.0	55800.0	55800.0	184974.6
Temp. (C)	482.0	25.0	20.0	20.0	482.2	25.0
Press. (KPA)	10300.0	102.0	10300.0	10300.0	10300.0	102.0

TABLE 2.4 (CONTINUED)

2.2.6 Discussion of Base Cases

2.2.6.1 Economic Comparison of the Base Cases

The table below is a breakdown of the installed capital cost for each base case, and Figure 2.5 is a comparison of the payback period for each plant based on the installed capital cost, operating costs, and any operating credits, with no discounting, taxes or other complications. The four base cases are the following:

Base Case 1 - Texaco Gasification and Steam Reformation

Base Case 2 - Lurgi Gasification

Base Case 3 - Steam Reformation Only

Base Case 4 - Texaco Gasification Only

(all costs in MM\$)	Case 1	Case 2	Case 3	Case 4
Cryogenic Oxygen Plant	76.7	139.9	-	82.6
Coal Preparation	47.7	91.9	-	51.8
Gasification	163.7	269.7	-	188.1
Slag Handling	3.0	5.9	-	3.3
Heat Recovery	7.8	-	-	8.4
Power Generation	89.3	166.7	51.5	83.1
Compressors	40.9	40.0	13.7	31.0
<hr/>				
Rectisol	38.2	121.9	18.7	41.1
Claus	11.1	21.5	-	12.0
Beavon	4.2	8.1	-	4.5
<hr/>				
Steam Reformer	16.8	-	62.5	-
Pressure Swing Adsorption	-	10.0	10.0	-
Sour Gas Shift Converter	-	-	-	6.7
<hr/>				
Alcohol Synthesis	40.0	40.0	40.0	40.0
CO ₂ Removal	15.6	15.6	15.6	15.6
Total	555.0	931.2	212.0	568.2

The four cases are described in more detail below and reasons for the differences in installed capital cost are given.

Gasification Blocks

Included in the syngas generation section are the Cryogenic Oxygen Plant, Coal Preparation, Gasification, Slag Handling, Heat Recovery (for 10000 kPa steam), Power Generation, and Compressors. The Cryogenic Oxygen Plant is included because the gasification requires the oxygen produced. Power Generation is

included because the change in cost is due mostly to the amount of coal-derived syngas produced. Compressors are included in this section because the change in their total cost is a function of the way in which the syngas is produced.

Case 1 and Case 4 economics are very similar, and they will be referred to as Case 1,4 unless a comparison between them is required. The cost of the Cryogenic Oxygen Plant is almost double in Case 2 over Case 1,4 because of the increased coal feed required. The Lurgi Gasification System produces value-added by-products, but as a consequence it also produces large amounts of CO_2 . Thus it is necessary to feed about three times as much coal to produce the same amount of syngas and, therefore, the same amount of mixed alcohols. For the same reason, the cost of the Coal Preparation, Gasification, and Slag Handling blocks are all similarly much higher. The above blocks, including the Cryogenic Oxygen Plant, are not required for Case 3. The heat recovery block is designed to produce 10000 kPa steam, which is only done in Case 1,4 because in Case 2 the gasification temperature is not high enough and in Case 3 no coal is gasified. The cost of the Power Generation block is a function of the gross power produced in this section, which is a function of the amount of methane produced in the process and the amount of 10000 kPa steam produced in the Heat Recovery block. A fixed amount of methane is generated in the Alcohol Synthesis Reactor, addition 10000 kPa steam is produced in the Case 1,4 Heat Recovery System, slightly increasing the cost, and in Case 2 a large amount of methane is produced in the Gasification Block which greatly increases the capital cost. The additional compressors in each plant are all roughly the same cost with the exception of Case 3 because no air compressor or oxygen compressor is required because no Cryogenic Oxygen Plant is required.

Acid Gas Cleanup and Sulfur Removal

The cost for the Rectisol block is largely a function of the CO_2 that must be removed. For this reason the cost of this block in Case 2 is far greater than the other blocks. Case 1,4 is next, while Case 3 is very low because the Steam Reformation system produces a much lower amount of CO_2 than either the Lurgi or the Texaco system. The cost of the Claus and Beavon Sulfur removal blocks is directly attributable to the amount of coal fed to the plant, so again, the Case 2 blocks are more expensive than the Case 1,4 blocks. Case 3 has no coal feed and thus no sulfur to remove.

Syngas H_2 :CO Ratio Adjustment

Case 1 requires a steam reformer to make a high H_2 :CO ratio gas to mix with the low ratio gas from the gasification block. Case 3 uses a reformer to generate all of its syngas and then removes the excess hydrogen with a Pressure Swing Adsorption block, as does Case 2 (The Lurgi gasifier produces a high H_2 :CO

PAYBACK PERIOD FOR WVUTASK2 BASE CASES

FIGURE 2.5

ratio gas because much of the C is converted to CO, instead of CO). Case 4 uses coal for its syngas generation so that a Sour Gas Shift Converter must be used to adjust the syngas ratio.

Alcohol Synthesis Loop

All four cases have the same feed to the Alcohol Synthesis Reactor. Consequently, the capital cost for all of the Cases is the same.

Summary

The Case 1 and Case 4 capital costs are almost the same because the coal feed to each of these cases is about the same. The Case 2 capital costs are much higher because much of the carbon feed to the Lurgi Gasifier is converted to species other than carbon monoxide. The Case 3 capital costs are much lower because the equipment need are less when natural gas is used as a feed stock.

2.2.7 Application of Simulated Annealing for Optimisation of Chemical Process Flowsheet

A background discussion on simulated annealing is given in Quarterly Technical Progress Report 5, January, 1993.

The production of higher alcohol fuels from syngas requires a separation block to create appropriate blends which can be used as fuel additives. This block consists of a train of distillation columns. The various distillation columns can have a wide variety of operating conditions depending on the requirements of the final product. However, this variation also leads to a wide fluctuation in the cost of the separation block. Thus, it is of great importance that the correct choice of operating conditions are used to obtain a good economical plant design.

Rigorous modeling of the distillation column can be done using RADFRAC block of ASPEN PLUS. The costing block of ASPEN PLUS provides the purchased cost of the distillation column. The cost for the condenser and the reboiler are also estimated for each set of operating conditions. These include the purchased cost of the equipment as well as the cost of utilities required on an annual basis. The various parameters which are considered as the variables are the composition of the feed stream, pressure profile in the column, feed stage location, degree of separation and the number of stages. The composition of the feed stream is considered a variable to incorporate the flexibility in the choice of the catalyst producing the alcohol. At present, the cost data has been generated and the application of simulated annealing to do the optimization is in progress. A FORTRAN code is being written to perform this optimization.

2.2.8 Economic Analysis

Preliminary investigations have focused primarily on cost reduction measures in stage 1 (syngas production) of the production process. While this work continues, the economic analysis has been expanded to encompass stage 2 (alcohol synthesis). Research activities in stage 2 include the modification of the spreadsheet model to provide a gate cost for the alcohol fuels and their market potential. The primary focus of the market research in this report is to determine the economic potential of butyl alcohol as blending agents or neat fuels.

Models

The spreadsheet model initially developed to determine the costs of syngas from the prospective sources has been modified in such a manner that a plant gate cost for the prospective alcohol fuels may be calculated. These costs may then be compared to the plant gate cost of gasoline to determine their current economic status. The future status of these fuels may also be determined by simply incorporating growth rates into the analysis. However, the value of these results are questionable, since they are likely to change due to modifications in the base cases. Once the base cases are complete, this model may provide an indication of the time frame in which coal derived alcohol fuels may become economical provided that they currently prove to be otherwise.

The original syngas cost model is currently being used to determine the economic constraints on capacity for the proposed facility. This should provide some indication as to the appropriate plant size enabling the facility to take advantage of economies of scale. Although it is clear that the capacity of the current base cases must be increased, the overall effect on the economic feasibility of coal derived syngas remains questionable. Increasing the capacity of these designs will inevitably result in the incorporation of additional gasifiers which in turn will significantly increase the capital cost. It remains to be seen if the increase in capital cost will be offset by the increases in syngas production to the point that the current economic status of these fuels changes.

Potential Cost Reducing Methods For Coal Derived Alcohol Fuels

Preliminary investigations suggest that the current economic status of coal derived alcohol fuels is questionable at best. However the potential to change this situation may lie in cost reducing measures. Technological advances will inevitably reduce capital cost in the future. Until this occurs, alternative cost reducing measures must be analyzed for any potential savings if these fuels are to be economically self-sufficient. Although there is a broad spectrum of potential by-products ranging from electric power to a vast array of value-added coal derivatives

commonly used as feedstocks for the chemical industry, the potential of by-products as an alternative to offset production costs appears to provide little potential. These markets appear to be limited with perhaps the exception electric power. For example, the demand for conventional coal derivatives has declined significantly over the years since many of these same products can be derived at a relatively lower cost from alternative feed stocks like oil. Consequently, these products provide a very limited capacity for reducing coal derived syngas cost. In fact, the production of by-products such as carbon dioxide and slag may even adversely effect the net cost of syngas if they have to be disposed of. Increasing environmental concerns necessitate the need to find potential markets for these products, in particular CO₂, to avoid the adverse effects of environmental policy issues like the proposed carbon tax.

One alternative to reduce the cost of alcohol fuels or syngas would be to use very inexpensive coal. Although the cost of coal is relatively small in contrast to the overall gasification cost, it does account for a significant portion of the annual operation cost therefore providing a significant cost saving opportunity. One source of inexpensive coal is old wash ponds. These ponds often contain significant amounts of coal left behind as a result of the coal preparation and cleaning process. This material could be fed into high temperature gasifiers in slurry form. The high operating temperatures of these gasifiers would essentially burn any combustible material and the remaining material would be discarded as slag. Coal refuse piles could also be another potential source of inexpensive coal for gasification. Although more expensive than the previous two sources, fine coal from continuous and long wall operations may also aid in this aspect of cost reduction. The coal from these operations could be screened and the fines used for gasification. This material could be purchased at a discount, since it would not have to go through the expensive cleaning process.

Another approach to reducing the cost may be obtained through an integrative approach of alcohol and electricity production. This integrative approach may provide a long needed low cost source of peaking power while simultaneously providing cost reducing capabilities for alcohol fuel production. Since methods of storing energy are limited or are expensive, peaking power must be provided by generating technologies rather than power storage technologies. The question is whether or not it would be possible to produce alcohol fuel or coal derived syngas in such a manner to take advantage of this situation. A major problem confronting the United States is how to most efficiently meet peak power demand both on a daily and on a seasonal basis. Currently, peaking plants often use natural gas fired turbines to provide peaking power requirements. Although capital requirements of these types of plants are low, plant utilization may be only 5 percent, significantly increasing the effective capital cost per kilowatt of power generated. Natural gas is also generally a more expensive fuel than coal for the generation

of electric power. As a result, peaking power is much more expensive than base-load power. However, if alcohol fuel plants were to produce more alcohol and less electricity at night, a portion of the alcohol produced during the night could be easily stored and burned during peak demand periods. This process would take advantage of the storage potential of alcohol thus providing relatively inexpensive means of storing power indirectly in order to meet peak demand. This arrangement would alleviate problems of using coal or natural gas for peaking power fuels in effect providing society with a low cost source of peaking power while simultaneously reducing the cost of clean burning alcohol fuels.

Alcohol Fuels Market

The exact composition of the mixed alcohol fuel has yet to be determined. However, it has been suggested that the desired alcohol product should be a butyl alcohol. Assuming that a butyl alcohol will be the major component of the mixed alcohol fuel, some insight may be gained into the potential demand for this fuel by examining the market for butyl alcohols in this capacity. Tertiary butyl alcohol's capacity as fuel additive was addressed in the report for the Forth Quarter of 1992; therefore, this will focus primarily on the remaining butyl alcohols.

Isobutanol was once considered to be an unwanted by-product generated in the production of oxo chemicals derived from propylene. This may explain in part its growth as fuel additive in the early 1980's. A number of companies under the United States Environmental Protection Agency's (EPA) Petrocoal waiver began to use alcohols as octane enhancers during this time period. Under this waiver, the addition of up to 15 volume percent alcohol could be used as a blending agent in gasoline. However, the composition of the alcohol was limited to a maximum 12 percent methanol and a maximum methyl to butyl alcohol ratio of 6.5 to 1. Consumption of isobutanol and n-butanol peaked under this waiver at approximately 9100 metric tons and 4500 metric tons respectively in 1983. After which, the market essentially collapsed due in part to the EPA's efforts to rescind the petrocoal waiver.

Continued growth in this industry has forced producers of oxo chemicals to rely on virtually any source of C₄ oxo molecules causing the conventional price spread between n-butanol and isobutanol to decrease significantly. As a result of this significant price inducement, isobutanol was adopted as a substitute for n-butanol in many markets. However, the overall tightening of C₄ feedstocks also decreased the economic viability of adding butanols to gasoline. Currently butanols are more valuable as chemical feedstocks than fuels; therefore, it is unlikely that these alcohols will be used as fuel given current oil prices. Estimates suggest that butanol may be economical if it can be produced at less than \$0.37 per liter provided that the pre tax gate cost of gasoline is in the range of \$ 0.19 to \$0.21 per liter.

Although the Petrocoal waiver permitting the use of butyl alcohols was revoked in 1984, legislation as of September 1990 permits the use of butanol as an octane enhancer. Currently aliphatic alcohols are limited to 2 percent oxygen by weight or 15 volume percent in the finished fuel with the exception of methanol. Since the fuel product is likely to be a blend of these various alcohols, it should be emphasized at this point that methanol appears to be an undesirable product from the stand point of EPA regulations. Therefore, to avoid complications of obtaining waivers for the use of this alcohol product, it may be advisable to eliminate methanol from the mixed alcohol fuel.

2.2.9 Fuels Evaluation

The three-pronged strategy adopted involves, (1) analysis of the blend characteristics (chemical and physical properties) using standard ASTM tests, (2) investigation of the performance characteristics on a single cylinder research engine and (3) investigation of the emissions characteristics.

2.2.9.1 Blend Characteristics

As a first step in the investigations of the emission and combustion characteristics of the fuel blends (gasoline and higher alcohols) with n-butanol properties such as energy density, octane number $((R + M)/2)$, water tolerance, flash point, API gravity, specific gravity distillation characteristics, stoichiometric air-to-fuel ratio, etc. will be determined. Initially, the C_4 alcohol that was to be employed was isobutanol. Using the equations given below, the stoichiometric air-to-fuel ratio can be determined for any type of blend.

The air-fuel ratio of indolene-alcohol blends can be calculated applying atom balance (Patel et al., 1987). The formula used for indolene is $C_{7.261}H_{13.87}$.

On molar basis ;

$$\begin{aligned} & \left[\frac{(1 - Y_M - Y_E - Y_P - Y_H)}{\bar{m}_I} \right] (C_{7.261}H_{13.87}) + \\ & \left[\frac{Y_M V^* \rho_m}{\bar{m}_M} \right] C H_3 OH + \left[\frac{Y_E V^* \rho_E}{\bar{m}_E} \right] C_2 H_5 OH + \\ & \left[\frac{Y_P V^* \rho_P}{\bar{m}_P} \right] C_3 H_7 OH + \left[\frac{Y_H V^* \rho_H}{\bar{m}_H} \right] C_4 H_9 OH \rightarrow a CO_2 + \\ & \quad b H_2 O + CO_2 + d N_2 \end{aligned}$$

Where:

y_I = volume fraction of indolene
 y_M = volume fraction of methanol
 y_E = volume fraction of ethanol
 y_P = volume fraction of propanol
 y_B = volume fraction of butanol

ρ_I = density of indolene = 0.74678 g/cm,
 ρ_M = density of methanol = 0.78959 g/cm,
 ρ_E = density of ethanol = 0.80761 g/cm,
 ρ_P = density of propanol = 0.80105 g/cm,
 ρ_B = density of butanol = 0.79955 g/cm,
 m = molecular weight
 V = volume

Taking atom balance, the final equation for air-fuel ratio at stoichiometric condition is

$$\left(\frac{A}{F}\right)_s = A/B$$

where

$$A = 1473.471 - 785.57065 y_M - 485.7355 y_E - 357.1806 y_P - 267.7698 y_B$$

$$B = 101.18082 + 5.80187 y_M + 8.24343 y_E + 7.3546 y_P + 7.18766 y_B$$

However, in this quarter the fuels evaluation group was informed that the molybdenum catalyst that is being used for alcohol synthesis can not yield isobutanol. Therefore, the straight chain alcohols, n-butanol will now be used.

Preliminary engine tests (gasoline-isobutanol blends) that were reported the last quarter have been discontinued. While limited information exists on work with isobutanol as a blending agent with gasoline practically no published literature, of value, could be found on the engine testing with n-butanol. Previous work on blends with isobutanol has been reviewed in earlier reports.

Schrock and Clark (1983) investigated the performance of n-butanol-acetone mixtures in a spark-ignition engine. The primary interest in determining the thermal efficiency and power of the engine as affected by mixture strength, and with a secondary emphasis on exhaust emissions. Engine tests showed that the mixture temperature averaged about 29 degrees lower for the blended fuel than for gasoline due to low stoichiometric ratio

and the high heat of vaporization of the two blended fuels. Exhaust temperature was 20 to 40 degrees cooler for the blends than for gasoline. The blends produce power and thermal efficiency roughly equivalent to gasoline. As the mixture is leaned in pursuit of higher thermal efficiency, power will decrease more for the blends than for gasoline.

Possible alcohol (higher alcohols plus methanol) blends were determined based on the levels of fuel oxygen. This estimate is based on iso-butanol. By varying the volume percentages of C_1 - C_4 alcohols three blends with 5% and 10% wt. oxygen were chosen for the process synthesis work. Tables 2.5 and 2.6 given below give the volume ratios of the alcohols for a two-fuel oxygen levels required. Oxygen levels were selected based on the allowable limit that the existing vehicles can handle given their air/fuel ratio control technology. The two specific levels, 5% and 10% wt. oxygen were originally used by Douthit and Talbot (1983).

Table 2.5

Alcohol Blends with 10% (% vol.) Isobutanol

PERCENT ISOBUTANOL (% volume)	PERCENT METHANOL (% volume)	PERCENT ETHANOL (% volume)	PERCENT PROPANOL (% volume)	TOTAL PERCENT OXYGEN (% weight)
10	1	4.5	3	5.027
10	1.5	5	1.5	5.05 "
10	0	2	8	4.99
10	0	4	5.5	5.02
10	7	6	8.5	10.01579
10	6	8	8	10.07812

Table 2.6 Alcohol Blends with 15% (% vol.) Isobutanol

PERCENT ISOBUTANOL (% volume)	PERCENT METHANOL (% volume)	PERCENT ETHANOL (% volume)	PERCENT PROPANOL (% volume)	TOTAL PERCENT OXYGEN (% weight)
15	1	1	3.5	5.024440
15	1.5	1.5	1.5	4.915035
15	1	1.5	2.5	4.931695
15	1.5	2	1.5	5.088950
15	1	2.5	1.5	5.012865
15	1	3	1	5.053450
15	5	4.5	10	9.975135
15	5	5	9.5	10.01572
15	5	5.5	9	10.05630
15	4.5	5.5	10	10.07296
15	5	6	8.5	10.09689
15	5	6.5	7.5	10.00414
15	4	6.5	9.5	10.03747
15	5	7	7	10.04473
15	4.5	7	8	10.06139
15	5	7.5	6.5	10.08531
15	4	7.5	8	9.985305
15	3	7.5	10	10.01863
15	4	8	7.5	10.02589
15	3	8	9	9.925880

2.2.9.2 Engine

A complete discussion of the test engine and data collection systems is contained in Quarterly Technical Progress Report 5, January, 1993.

2.2.9.3 Combustion Characteristics

In addition to measuring the emissions characteristics of the fuel blends effort will be devoted to investigation of the ignition delay and flame speeds over a wide range of compression ratios. Following the procedures outlined in the last report the engine will be tested on a dyno. An induction probe will be used to determine the flame speeds inside the cylinder. The burning velocity is equal to the difference between the flame speed and the transport velocity of the unburned gases normal to and away from the front. While the flame speed is measured using the ionization probe, the transport velocity is due to the piston motion and the expansion of burned gases. The burning velocity is calculated from an equation developed by Chaibongsai (1980).

$$S_u = S_b - S_g$$

$$S_u = S_b - \frac{V_u}{A_f n P} \frac{dp}{dt} - \frac{V_u}{A_f V_t} \frac{dV_t}{dt}$$

Where ;

S_b = flame speed

S_u = actual turbulent burning velocity

S_g = transport velocity

V_u = cylinder volume occupied by unburnt gas portion

V_t = total cylinder volume

A_f = frontal area

P = pressure

n = polytropic exponent

Layout of Instrumentation

FIGURE 2.6

Prediction of performance and emissions from gasoline-higher alcohol fueled engines is possible by making several over simplifying assumptions as has been done by researchers in the past who have developed semi-empirical models. A brief discussion on the calculation of the laminar burning velocities is given below.

Theoretical prediction of the laminar and turbulent burning velocity requires a solution of the continuity, momentum and energy equations coupled with chemical kinetics of the basic reactions involved in combustion process. Laminar burning velocity depends on the cylinder pressure, equivalence ratio, residual gas fraction, the unburned mixture temperature, etc. However, this complicated process can be resolved by calculating the laminar burning velocity calculated using Semenov's equation for the burning velocity in a combustible mixture as given below (Patel and Henein, 1986). The adiabatic flame temperature is calculated assuming chemical equilibrium of the products of combustion (Olikara and Borman, 1975).

$$S_l = \left[\frac{2\lambda_f k a_o c_{pf}^2}{\rho_i C_3} \left(\frac{T_i}{T_f} \right)^n \left(\frac{\lambda_v}{C_{pf} \rho_v D_v} \right)^n \left(\frac{N_1}{N_2} \right) \right. \\ \left. (RT_f)^2 \left(\frac{RT_f^2}{E} \right)^{n+1} \frac{e^{-E/RT_f}}{(T_f - T_i)^{n+1}} \right]^{1/2}$$

where ;

k = global rate for all oxidation reactions

a_o = number of molecules per unit volume of combustible in initial mixture

C_{pf} = specific heat at T_f

C_p = average specific heat at T_i and T_f

D_v = Diffusivity at T_v

E = activation energy

N_1 = moles of reactants

N_2 = moles of products

R = gas Constant

T_i = initial temperature

T_f = flame temperature

λ_v = thermal Conductivity at T_v

λ_f = thermal Conductivity at T_i

ρ_v = density at T_v

ρ_i = density at T_i

Metghalchi and Keck (1982) investigated the laminar burning velocity in methanol-air and indolene-air mixtures, in a constant volume bomb. Using the equation by Metghalchi and Keck (1982) the laminar burning velocity of the unburned mixture can be calculated (at any temperature and pressure):

$$\frac{S_l}{S_o} = \left(\frac{T_u}{T_o} \right)^\alpha \left(\frac{P}{P_o} \right)^\beta (1 - 2.1f)$$

Where ;

- α = 2.19
- β = -0.13 .
- S_l = Laminar burning velocity
- T_u = Unburnt gas temperature
- T_o = Reference temperature
- P = Pressure
- P_o = Reference pressure
- f = Residual gas fraction

By considering the reaction rate constants of the individual fuel-air mixtures the value of K can be calculated in order to determine the laminar burning velocity of the gasoline-higher alcohol blend.

$$K = x_1 K_1 + x_2 K_2$$

Where ; K, K_1 and K_2 = Reaction rate constants

Also, as reported by Patel and Henein (1986) the laminar burning velocity can be calculated from the individual burning velocities and their mole fraction in the blends

$$S_{lo} = x_1 (S_{lo})_1 + x_2 (S_{lo})_2$$

Where S_{lo} = Laminar burning velocity at 1 atm pressure, 298°K temperature and pure fuel.

2.2.9.4 Corrosion

The corrosivity of alcohol fuels, has been studied extensively by several researchers. Of particular interest in this quarter was the history of methyl formate and methyl acetate which are a by-product of the alcohol synthesis process. In the presence of water, methyl formate will hydrolyze to form formic acid and methanol. The hydrolyzing rate depends on the temperature and on the presence of acid (H^+). The higher the temperature, the faster the hydrolyzing rate. At very low temperatures (freezing) hydrolysis will not occur. Formic acid is corrosive because of the acidic behaviour. Methyl formate is soluble in about 3.3 parts water and is miscible with alcohol. Methyl acetate will hydrolyze to form acetic acid and methanol. The hydrolyzing rate of methyl acetate is slower than that of methyl formate. Methyl acetate is soluble in water, and is miscible in alcohol. Methanol which is a byproduct of the hydrolysis also causes corrosion problems with certain metals. Dry methanol-gasoline blends will corrode magnesium within hours because of the formation of magnesium methoxide. The presence of water tends to form an insoluble magnesium hydroxide coating on the metal and this helps prevent corrosion.

The next step in the project is to blend mixtures of n-butanol, propanol, ethanol and methanol and have the blends analyzed in a standard ASTM lab. The data acquisition system will be assembled and connected to the engine before any tests will be run.

2.3 Conclusions and Recommendations

2.4 Future Plans

The next step in the fuels evaluation part of the project is to blend mixtures of n-butanol, propanol, ethanol and methanol and have the blends analyzed in a standard ASTM lab. The data acquisition system will be assembled and connected to the engine before any tests will be run.

2.5 Appendices for Task 2

2.5.1 Appendix 2-1

SYNGAS PRODUCTION FROM NATURAL GAS

Compressed natural gas (stream 14) and steam (stream 15) are reacted in the Steam Reformation Block. The cooled output gas (stream 17) goes to the Rectisol Block. The cost for this unit was estimated from data found for a hydrogen production facility (2).

Installed Capital Cost (1992 dollars) = \$16.8 MM

COAL PREPARATION

Coal (stream 10), limestone (stream 11), and water (stream 12), are sent to the Coal Preparation Block. The coal and limestone are crushed, mixed with the water, and pumped to the gasifier as a 70% solids mixture by weight (stream 13). The Coal Preparation Block is comprised of five plants from the Houston report. Plant 01 is the Coal Slurry Preparation Plant. The cost of this plant was scaled linearly to its multiple train format and includes two trains plus one spare compared to eight trains plus two spares for the Houston system. Plant 61 is the Reclaiming, Transfer, and Crushing Plant. The cost of this plant was scaled exponentially. Plant 22 is the Barge Terminal. This plant was scaled exponentially. Plant 60 is Coal Receiving and Storage and again the cost for this plant was scaled exponentially. Plant 65 is the Limestone Handling Facility. The cost of this plant is assumed to be the same as the Houston report for the base case.

Power needs = 1.9 MW

Installed Capital Cost (1992 dollars) = \$47.7 MM

CRYOGENIC OXYGEN PLANT

Compressed air (stream 1) is cooled and sent to the Cryogenic Oxygen Plant Block, and is separated into high purity oxygen (stream 2), nitrogen (stream 3), argon (stream 6), other rare gases (stream 7), and a water and carbon dioxide waste mixture (stream 28). A small quantity of nitrogen (stream 19) is sent to the Rectisol Block. The Cryogenic Oxygen Plant Block does not include the inlet air compressors or the outlet oxygen compressors, but it does include a refrigeration system that serves the needs of the entire base case. The Houston system uses four trains of cryogenic oxygen production and two trains plus one spare of refrigeration. In the cryogenic system, there are provisions for gaseous and liquid oxygen backups sufficient to maintain downstream plant operation in the event of a shutdown in the cryogenic facility. Since our needs are approximately 25 percent that of the Houston system, we assume that only one cryogenic train will be necessary. As for the refrigeration system, we assume that one train plus one spare will be

sufficient. We also assume that some scale down is possible for this system, so the capital investment has been calculated linearly for the reduction in trains, and exponentially for throughput reduction per train. The Houston plants which comprise the Cryoplant Block are 02 and 08.

Power needs = 0.0

Steam needs = 700 kg/hr, 1700 kPa, 250°C

Installed Capital Cost (1992 dollars) = \$76.7 MM

RECTISOL

The cooled raw gas streams (streams 17 and 18), nitrogen gas (stream 19) for methanol regeneration, and methanol make-up (stream 20) for vapor loss all enter the Rectisol Block. H₂S levels are reduced to the ppb range and CO₂ levels to the ppm range. The bulk of the clean syngas (stream 22) is sent to the alcohol synthesis loop while 1% (stream 25) is sent to the COS Hydrolysis Block. A CO, N₂ mixture (stream 24) and a CO₂ rich stream (stream 23) are produced as byproducts. Condensed water is also removed (stream 17A). This block is the same as Houston Plant 05. The cost for this plant was estimated by using linear and exponential scaling.

Power needs = 1.0 MW

Steam needs = 1500 kg/hr, saturated, 200 kPa

11000 kg/hr, 350 kPa, 130°C

Installed Capital Cost (1992 dollars) = \$38.2 MM

TEXACO GASIFIER

The coal slurry (stream 13) is mixed with compressed oxygen (stream 9) and burned at 1200-1400°C and 8000 kPa in the Texaco Gasifier Block. The hot, raw gas (stream 8) is sent to the Syngas Heat Recovery Block, and the slag (stream 33) is sent to the Slag Handling Block. The Houston system uses ten trains of gasifiers with two of the ten as spares. Our base case calls for a coal feed approximately one quarter that of the Houston Plant. Thus, we assume that our plant will require two trains plus one spare train, and the capital cost will be thirty percent that of the Houston system. The equivalent of the Texaco Gasifier Block is Plant 03 in the Houston report.

Power needs = 0.5 MW

Steam needs = 6000 kg/hr, 350 kPa, 130°C

Installed Capital Cost (1992 dollars) = \$163.7 MM

SLAG HANDLING

Molten slag from the Texaco Gasifier Block (stream 33) is direct quenched with water and sent to slag disposal (stream 37). A small amount of water (stream 36) is purged from the closed loop and is replaced by water make-up (stream 34). This block is the same as Houston Plant 63. The cost for this plant was

estimated by exponential scaling.

Power needs = 0.0

Installed Capital Cost (1992 dollars) = \$3.0 MM

COS HYDROLYSIS

The sulfide rich stream from the Rectisol Block (stream 25), a small stream of clean syngas (stream 38), and air (stream 39) are sent to the COS Hydrolysis Block where COS is converted to H_2S . The product gas (stream 41) is sent to the Claus Sulfur Recovery Block. The COS Hydrolysis Block may actually be a small part of the Rectisol Block, but in any case, its cost is assumed to be negligible.

SYNGAS HEAT RECOVERY

The raw gas stream from the Texaco Gasifier Block (stream 8) at $1200^{\circ}C$ and 8000 kPa enters the Syngas Heat Recovery Block and is cooled against process boiler feed water at $15^{\circ}C$ (stream 71). The raw gas stream exits at $300^{\circ}C$ (stream 18), and the boiler feed exits as steam at 10000 kPa and $450^{\circ}C$ (stream 68). It is assumed that the raw gas stream is cooled further prior to entering the Rectisol Block. This block is part of Houston Plant 04, which includes heat recovery and gas shifting for part of the feed. It was assumed that one syngas cooling train was approximately equal to one-sixth of the total cost of Houston Plant 04. The cost of the two cooling trains was then scaled exponentially.

Heat removed = 4.44×10^8 kJ/hr

Power needs = 0.4 MW

Installed Capital Cost (1992 dollars) = \$7.8 MM

CLAUS PLANT

Hydrogen sulfide rich gas (stream 41) is mixed with air (stream 42) and converted in a two step reaction to elemental sulfur (stream 46). The unreacted hydrogen sulfide (stream 45) is then sent to the Beavon Plant for further treatment. This block is the same as Houston Plant 06. The cost for this plant was estimated by exponential scaling.

Power needs = 0.2 MW

Steam needs = 6000 kg/hr, saturated, 4500 kPa

5000 kg/hr, 1700 kPa, $250^{\circ}C$

Installed Capital Cost (1992 dollars) = \$11.1 MM

BEAVON PLANT

The Claus tail gas (stream 45), air (stream 47), and water (stream 48) all go to the Beavon Block. Additional sulfur is made (stream 51), and the gas leaving (stream 50) is sufficiently free from sulfides that it can be vented to the atmosphere. A sour water stream (stream 54) is sent from the plant for treatment. The cost of this block was estimated from data collected from various sources (3).

Installed Capital Cost (1992 dollars) = \$4.2 MM

MOB, ALCOHOL SYNTHESIS LOOP

Clean syngas (stream 26) at 140 atmospheres enters the catalytic reactor along with the syngas recycle (stream 56B). The products (stream 26A) are taken to the separations block where the unreacted syngas is removed (stream 59). Part of this stream (stream 27) is sent to power generation while the rest (stream 56) is sent to CO₂ removal. The cost of this block was estimated from the cost of a methanol synthesis loop (4).

Installed Capital Cost (1992 dollars) = \$40.0 MM

CO₂ REMOVAL

This block is very similar to the Rectisol Block. Recycled gas from the alcohol separation block (stream 56) is the only feed. CO₂ free syngas (stream 56A) is then recompressed and sent back to the reactor. CO₂ is taken off as a product (stream 57). The cost of this block is assumed to be an exponential function of the Rectisol block.

Installed Capital Cost (1992 dollars) = \$15.6 MM

STEAM/POWER GENERATION

10% of the unreacted syngas from the Alcohol Synthesis Loop (stream 27) is letdown in a turbine and then saturated with water (stream 65). This water vapor helps prevent the formation of NO_x compounds when this stream (stream 70) is then burned with air (stream 67) to provide heat for 10000 kPa, 450°C steam production. This steam (stream 74) is mixed with steam of the same type from the Syngas Heat Recovery block and let down in the steam turbines for power production. As a gross estimate, the four blocks, Syngas Saturation, Gas Turbine, Combuster, and Steam Turbines, as well as other needs in this category not shown on the flowsheet, are assumed to fall within Houston plant 31. The power rating on the Houston steam turbines is 60 MW, and the load on our turbines is 96 MW. The cost for these blocks was determined by exponential scaling.

Power produced = 96 MW

Installed Capital Cost (1992 dollars) = \$89.3 MM

2.5.2 Appendix 2-2 Base Case 2 Lurgi Gasifier Plus Natural Gas

COAL PREPARATION

Coal (stream 10), limestone (stream 11), and water (stream 12), are sent to the Coal Preparation Block. The coal and limestone are crushed, mixed with the water, and pumped to the gasifier (stream 13). The Coal Preparation Block is comprised of five plants from the Houston report. Plant 01 is the Coal Slurry Preparation Plant. The cost of this plant was scaled linearly to its multiple train format and includes five trains plus two spares compared to eight trains plus two spares for the Houston system. Plant 61 is the Reclaiming, Transfer, and Crushing Plant. The cost of this plant was scaled exponentially. Plant 22 is the Barge Terminal. This plant was scaled exponentially. Plant 60 is Coal Receiving and Storage and again the cost for this plant was scaled exponentially. Plant 65 is the Limestone Handling Facility. The cost of this plant is assumed to be the same as the Houston report for the base case.

Power needs = 5.2 MW

Installed Capital Cost (1992 dollars) = \$91.9 MM

LURGI GASIFIER

The coal slurry (stream 13) is mixed with compressed oxygen (stream 9) and burned at 400°C and 8000 kPa in the Lurgi Gasifier Block. The hot, raw gas (stream 8) is sent to the Syngas Heat Recovery Block, and the slag (stream 33) is sent to the Slag Handling Block. Economic data for this block was obtained from a report on the Great Plains Gasification Project. (Miller, W.R. and R.A. Lang, "Great Plains Coal Gasification Plant Public Design Report," Volume 1, DOE/CH/10088-1874-Vol.1, July, 1985.)

Power needs = 1.3 MW

Steam needs = 13000 kg/hr, 350 kPa, 130 °C

Installed Capital Cost (1992 dollars) = \$269.7 MM

SLAG HANDLING

Molten slag from the Lurgi Gasifier Block (stream 33) is directly quenched with water and sent to slag disposal (stream 37). A small amount of water (stream 36) is purged from the closed loop and is replaced by water make-up (stream 34). This block is the same as Houston Plant 63. The cost for this plant was estimated by exponential scaling.

Power needs = 0.0

Installed Capital Cost (1992 dollars) = \$5.9 MM

CRYOGENIC OXYGEN PLANT

Compressed air (stream 1) is cooled and sent to the Cryogenic Oxygen Plant Block, and is separated into high purity oxygen (stream 2), nitrogen (stream 3), argon (stream 6), other rare

gases (stream 7), and a water and carbon dioxide waste mixture (stream 28). A small quantity of nitrogen (stream 19) is sent to the Rectisol Block. The Cryogenic Oxygen Plant Block does not include the inlet air compressors or the outlet oxygen compressors, but it does include a refrigeration system that serves the needs of the entire base case. The Houston system uses four trains of cryogenic oxygen production and two trains plus one spare of refrigeration. In the cryogenic system, there are provisions for gaseous and liquid oxygen backups sufficient to maintain downstream plant operation in the event of a shutdown in the cryogenic facility. Since our needs are slightly less than 50 percent that of the Houston system, we assume that only two cryogenic trains will be necessary. As for the refrigeration system, we assume that one train plus one spare will be sufficient. The capital investment has been calculated linearly for the reduction in trains, and exponentially for throughput change per train. The Houston plants which comprise the Cryoplant Block are 02 and 08.

Power needs = 0.0

Steam needs = 1200 kg/hr, 1700 kPa, 250°C

Installed Capital Cost (1992 dollars) = \$139.9 MM

COS HYDROLYSIS

The sulfide rich stream from the Rectisol Block (stream 25), a small stream of clean syngas (stream 38), and air (stream 39) are sent to the COS Hydrolysis Block where COS is converted to H_2S . The product gas (stream 41) is sent to the Claus Sulfur Recovery Block. The COS Hydrolysis Block may actually be a small part of the Rectisol Block, but in any case, its cost is assumed to be negligible.

RECTISOL

The cooled raw gas stream (stream 18), nitrogen gas (stream 19) for methanol regeneration, and methanol make-up (stream 20) for vapor loss all enter the Rectisol Block. H_2S levels are reduced to the ppb range and CO levels to the ppm range. The bulk of the clean syngas (stream 22) is sent to the alcohol synthesis loop while 1% (stream 25) is sent to the COS Hydrolysis Block. A CO_2 , N_2 mixture (stream 24) and a CO rich stream (stream 23) are produced as byproducts. Condensed water is also removed (stream 17A). This block is the same as Houston Plant 05. The cost for this plant was estimated by using linear and exponential scaling.

Power needs = 5.9 MW

Steam needs = 8000 kg/hr, saturated, 700 kPa

60000 kg/hr, 350 kPa, 130°C

Installed Capital Cost (1992 dollars) = \$121.9 MM

CLAUS PLANT

Hydrogen sulfide rich gas (stream 41) is mixed with air (stream

42) and converted in a two step reaction to elemental sulfur (stream 46). The unreacted hydrogen sulfide (stream 45) is then sent to the Beavon Plant for further treatment. This block is the same as Houston Plant 06. The cost for this plant was estimated by exponential scaling.

Power needs = 0.6 MW

Steam needs = 15000 kg/hr, saturated, 4500 kPa

11000 kg/hr, 1700 kPa, 530°F

Installed Capital Cost (1992 dollars) = \$21.5 MM

BEAVON PLANT

The Claus tail gas (stream 45), air (stream 47), and water (stream 48) all go to the Beavon Block. Additional sulfur is made (stream 51), and the gas leaving (stream 50) is sufficiently free from sulfides that it can be vented to the atmosphere. A sour water stream (stream 54) is sent from the plant for treatment. The cost of this block was estimated from data collected from various sources (2).

Installed Capital Cost (1992 dollars) = \$8.1 MM

MOS, ALCOHOL SYNTHESIS LOOP

Clean syngas (stream 26) at 140 atmospheres enters the catalytic reactor along with the syngas recycle (stream 56B). The products (stream 26A) are taken to the separations block where the unreacted syngas is removed (stream 59). Part of this stream (stream 27) is sent to power generation while the rest (stream 56) is sent to CO₂ removal. The cost of this block was estimated from the cost of a methanol synthesis loop (3).

Installed Capital Cost (1992 dollars) = \$40.0 MM

CO₂ REMOVAL

This block is very similar to the Rectisol Block. Recycled gas from the alcohol separation block (stream 56) is the only feed. CO₂ free syngas (stream 56A) is then recompressed and sent back to the reactor. CO₂ is taken off as a product (stream 57). The cost of this block is assumed to be an exponential function of the Rectisol block.

Installed Capital Cost (1992 dollars) = \$15.6 MM

STEAM/POWER GENERATION

Methane and ethane generated in the process (stream 27) are let down in a turbine and then saturated with water (stream 65). This water vapor helps prevent the formation of NO_x compounds when this stream (stream 70) is then burned with air (stream 67) to provide heat for 10000 kPa, 450°C steam production. This steam (stream 74) is then let down in the steam turbines for power

production. As a gross estimate, the four blocks, Syngas Saturation, Gas Turbine, Combuster, and Steam Turbines, as well as other needs in this category not shown on the flowsheet, are assumed to fall within Houston plant 31. The power rating on the Houston steam turbines is 60 MW, and the load on our turbines is 209 MW. It is assumed that the cost for these blocks can be exponentially scaled from Houston plant 31.

Power needs = 209 MW

Installed Capital Cost (1992 dollars) = \$166.7 MM

PRESSURE SWING ADSORPTION

The clean syngas (stream 22A) is sent to PSA for selective hydrogen removal and purification. The adjusted syngas (stream 22AA) is sent on to the reactor while the purified excess hydrogen is sent to the plant battery limits for sale if possible. The flowrates between this case and the Houston report are fairly equal, so the power usage and installation costs are assumed to be roughly equal.

Power needs = 0.1 MW

Installed Capital Cost (1992 dollars) = \$10.0 MM

2.5.3 Appendix 2-3

SYNGAS PRODUCTION FROM NATURAL GAS

Compressed natural gas (stream 14) and steam (stream 15) are reacted in the Steam Reformation Block. The cooled output gas (stream 17) goes to the Rectisol Block. The cost for this unit was estimated from data found for a hydrogen production facility (2).

Installed Capital Cost (1992 dollars) = \$62.5 MM

RECTISOL

The cooled gas stream (stream 17) , nitrogen gas (stream 19) for methanol regeneration, and methanol make-up (stream 20) for vapor loss all enter the Rectisol Block. CO₂ levels are reduced to the ppm range. The clean syngas (stream 22) is sent to the alcohol synthesis loop. A CO₂, N₂ mixture (stream 24) and a CO₂ rich stream (stream 23) are produced as byproducts. Condensed water is also removed (stream 17A). This block is the same as Houston Plant 05. The cost for this plant was estimated by using linear and exponential scaling.

Installed Capital Cost (1992 dollars) = \$18.7 MM

PRESSURE SWING ADSORPTION

The clean syngas (stream 22A) is sent to PSA for selective hydrogen removal and purification. The adjusted syngas (stream 22AA) is sent on to the reactor while the purified excess hydrogen is sent to the plant battery limits for sale if possible.

Installed Capital Cost (1992 dollars) = \$10.0 MM

MoS₂ ALCOHOL SYNTHESIS LOOP

Clean syngas (stream 26) at 140 atmospheres enters the catalytic reactor along with the syngas recycle (stream 56B). The products (stream 26A) are taken to the separations block where the unreacted syngas is removed (stream 59). Part of this stream (stream 27) is sent to power generation while the rest (stream 56) is sent to CO₂ removal. The cost of this block was estimated from the cost of a methanol synthesis loop (3).

Installed Capital Cost (1992 dollars) = \$40.0 MM

CO₂ REMOVAL

This block is very similar to the Rectisol Block. Recycled gas from the alcohol separation block (stream 56) is the only feed. CO₂ free syngas (stream 56A) is then recompressed and sent back to the reactor. CO₂ is taken off as a product (stream 57). The cost

of this block is assumed to be an exponential function of the Rectisol block.

Installed Capital Cost (1992 dollars) = \$15.6 MM

STEAM/POWER GENERATION

Methane and ethane are letdown in a turbine and then saturated with water (stream 65). This water vapor helps prevent the formation of NO_x compounds when this stream (stream 70) is then burned with air (stream 67) to provide heat for 100 kPa, 400°C steam production. This steam (stream 74) is then let down in the steam turbines for power production. As a gross estimate, the four blocks, Syngas Saturation, Gas Turbine, Combuster, and Steam Turbines, as well as other needs in this category not shown on the flowsheet, are assumed to fall within Houston plant 31.

Power needs = 44 MW

Installed Capital Cost (1992 dollars) = \$51.5 MM

2.5.4 Appendix 2-4

COAL PREPARATION

Coal (stream 10), limestone (stream 11), and water (stream 12), are sent to the Coal Preparation Block. The coal and limestone are crushed, mixed with the water, and pumped to the gasifier as a 70% solids mixture by weight (stream 13). The Coal Preparation Block is comprised of five plants from the Houston report. Plant 01 is the Coal Slurry Preparation Plant. The cost of this plant was scaled linearly to its multiple train format and includes three trains plus one spare compared to eight trains plus two spares for the Houston system. Plant 61 is the Reclaiming, Transfer, and Crushing Plant. The cost of this plant was scaled exponentially. Plant 22 is the Barge Terminal. This plant was scaled exponentially. Plant 60 is Coal Receiving and Storage and again the cost for this plant was scaled exponentially. Plant 65 is the Limestone Handling Facility. The cost of this plant is assumed to be the same as the Houston report for the base case.

Power needs = 2.1 MW

Installed Capital Cost (1992 dollars) = \$51.8 MM

TEXACO GASIFIER

The coal slurry (stream 13) is mixed with compressed oxygen (stream 9) and burned at 1200-1400°C and 8000 kPa in the Texaco Gasifier Block. The hot, raw gas (stream 8) is sent to the Syngas Heat Recovery Block, and the slag (stream 33) is sent to the Slag Handling Block. The Houston system uses ten trains of gasifiers with two of the ten as spares. Our base case calls for a coal feed approximately one third that of the Houston Plant. Thus, we assume that our plant will require three trains plus one spare train, and the capital cost will be forty percent that of the Houston system. The equivalent of the Texaco Gasifier Block is Plant 03 in the Houston report.

Power needs = 0.5 MW

Steam needs = 6000 kg/hr, 350 kPa, 130°C

Installed Capital Cost (1992 dollars) = \$188.1 MM

CRYOGENIC OXYGEN PLANT

Compressed air (stream 1) is cooled and sent to the Cryogenic Oxygen Plant Block, and is separated into high purity oxygen (stream 2), nitrogen (stream 3), argon (stream 6), other rare gases (stream 7), and a water and carbon dioxide waste mixture (stream 28). A small quantity of nitrogen (stream 19) is sent to the Rectisol Block. The Cryogenic Oxygen Plant Block does not include the inlet air compressors or the outlet oxygen compressors, but it does include a refrigeration system that serves the needs of the entire base case. The Houston system uses four trains of cryogenic oxygen production and two trains plus one spare of refrigeration. In the cryogenic system, there are provisions for gaseous and liquid oxygen backups sufficient

to maintain downstream plant operation in the event of a shutdown in the cryogenic facility. Since our needs are approximately 35 percent that of the Houston system, we assume that only one cryogenic train will be necessary. As for the refrigeration system, we assume that one train plus one spare will be sufficient. We also assume that some scale down is possible for this system, so the capital investment has been calculated linearly for the reduction in trains, and exponentially for throughput reduction per train. The Houston plants which comprise the Cryoplant Block are 02 and 08.

Power needs = 0.0

Steam needs = 800 kg/hr, 1700 kPa, 250°C

Installed Capital Cost (1992 dollars) = \$82.6 MM

RECTISOL

The cooled raw gas stream (stream 18) , nitrogen gas (stream 19) for methanol regeneration, and methanol make-up (stream 20) for vapor loss all enter the Rectisol Block. H₂S levels are reduced to the ppb range and CO₂ levels to the ppm range. The bulk of the clean syngas (stream 22) is sent to the alcohol synthesis loop while 1% (stream 25) is sent to the COS Hydrolysis Block. A CO₂, N₂ mixture (stream 24) and a CO₂ rich stream (stream 23) are produced as byproducts. Condensed water is also removed (stream 17A). This block is the same as Houston Plant 05. The cost for this plant was estimated by using linear and exponential scaling.

Power needs = 1.1 MW

Steam needs = 1600 kg/hr, saturated, 700 kPa

11000 kg/hr, 350 kPa , 130°C

Installed Capital Cost (1992 dollars) = \$41.1 MM

SLAG HANDLING

Molten slag from the Texaco Gasifier Block (stream 33) is direct quenched with water and sent to slag disposal (stream 37). A small amount of water (stream 36) is purged from the closed loop and is replaced by water make-up (stream 34). This block is the same as Houston Plant 63. The cost for this plant was estimated by exponential scaling.

Power needs = 0.0

Installed Capital Cost (1992 dollars) = \$3.3 MM

COS HYDROLYSIS

The sulfide rich stream from the Rectisol Block (stream 25), a small stream of clean syngas (stream 38), and air (stream 39) are sent to the COS Hydrolysis Block where COS is converted to H₂S. The product gas (stream 41) is sent to the Claus Sulfur Recovery Block. The COS Hydrolysis Block may actually be a small part of the Rectisol Block, but in any case, its cost is assumed to be

negligible.

SYNGAS HEAT RECOVERY

The raw gas stream from the Texaco Gasifier Block (stream 8) at 1200°C and 8000 kPa enters the Syngas Heat Recovery Block and is cooled against process boiler feed water at 15°C (stream 71). The raw gas stream exits at 300°C (stream 18), and the boiler feed exits as steam at 10000 kPa and 450°C (stream 68). It is assumed that the raw gas stream is cooled further prior to entering the Rectisol Block. This block is part of Houston Plant 04, which includes heat recovery and gas shifting for part of the feed. It was assumed that one syngas cooling train was approximately equal to one-sixth of the total cost of Houston Plant 04. The cost of the two cooling trains was then scaled exponentially.

Power needs = 0.4 MW

Installed Capital Cost (1992 dollars) = \$8.4 MM

CLAUS PLANT

Hydrogen sulfide rich gas (stream 41) is mixed with air (stream 42) and converted in a two step reaction to elemental sulfur (stream 46). The unreacted hydrogen sulfide (stream 45) is then sent to the Beavon Plant for further treatment. This block is the same as Houston Plant 06. The cost for this plant was estimated by exponential scaling.

Power needs = 0.3 MW

Steam needs = 6000 kg/hr, saturated , 4500 kPa

5000 kg/hr, 1700 kPa, 250°C

Installed Capital Cost (1992 dollars) = \$12.0 MM

BEAVON PLANT

The Claus tail gas (stream 45), air (stream 47), and water (stream 48) all go to the Beavon Block. Additional sulfur is made (stream 51), and the gas leaving (stream 50) is sufficiently free from sulfides that it can be vented to the atmosphere. A sour water stream (stream 54) is sent from the plant for treatment. The cost of this block was estimated from data collected from various sources (2).

Installed Capital Cost (1992 dollars) = \$4.5 MM

MoS₂ ALCOHOL SYNTHESIS LOOP

Clean syngas (stream 26) at 140 atmospheres enters the catalytic reactor along with the syngas recycle (stream 56B). The products (stream 26A) are taken to the separations block where the unreacted syngas is removed and recycled (stream 59). The methane and ethane generated in the reaction (stream 27) is sent to power generation while the recycled syngas (stream 56) is

sent to CO₂ removal. The cost of this block was estimated from the cost of a methanol synthesis loop (3).

Installed Capital Cost (1992 dollars) = \$40.0 MM

CO₂ REMOVAL

This block is very similar to the Rectisol Block. Recycled gas from the alcohol separation block (stream 56) is the only feed. CO₂ free syngas (stream 56A) is then recompressed and sent back to the reactor. CO₂ is taken off as a product (stream 57). The cost of this block is assumed to be an exponential function of the Rectisol block.

Installed Capital Cost (1992 dollars) = \$15.6 MM

STEAM/POWER GENERATION

Methane and ethane generated in the process (stream 27) is letdown in a turbine and then saturated with water (stream 65). This water vapor helps prevent the formation of NO_x compounds when this stream (stream 70) is then burned with air (stream 67) to provide heat for 10000 kPa, 450°C steam production. This steam (stream 74) is mixed with steam of the same type from the Syngas Heat Recovery block and let down in the steam turbines for power production. As a gross estimate, the four blocks, Syngas Saturation, Gas Turbine, Combuster, and Steam Turbines, as well as other needs in this category not shown on the flowsheet, are assumed to fall within Houston plant 31. The power rating on the Houston steam turbines is 60 MW, and the load on our turbines is 86 MW. The cost for these blocks was determined by exponential scaling.

Power needs = 86.0 MW

Installed Capital Cost (1992 dollars) = \$83.1 MM

SOUR GAS SHIFT CONVERTER

Raw fuel gas (stream 8A) leaving the Heat Recovery Block is shifted to produce the desired H₂ to CO ratio needed in the alcohol synthesis reactor.

Installed Capital Cost = \$6.7 MM

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