QUARTERLY TECHNICAL PROGRESS REPORT
NUMBER 5

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

CONTRACT NO. DE-AC22-91PC91034

REPORTING PERIOD:

October 1, 1992 to December 31, 1992

SUBMITTED TO:

Document Control Center
U.S. Department of Energy
Pittsburgh Energy Technology Center
P.O. Box 10940, MS 921-118
Pittsburgh, PA 15236-0940

SUBMITTED BY:

West Virginia University Research Corporation
on behalf of West Virginia University
213 Glenlock Hall
Morgantown, WV 26506

January, 1993

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

U.S. DOE Patent Clearance is not required prior to the publication of this document.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

TABLE OF CONTENTS

TASK 1 REACTION STUDIES

.... 1.1 LABORATORY SETUP	1
.... 1.2 CATALYST RESEARCH	2
.... TABLE 1. EFFECT OF IMPREGNATION ORDER ON O ₂ CHEMISORPTION WITH Mo-Co/C CATALYSTS	3
.... 1.3 REACTOR ENGINEERING	3

TASK 2 PROCESS SYNTHESIS AND FUEL EVALUATION

.... EXECUTIVE SUMMARY	6
------------------------------	---

APPENDIX 1

.... BASE CASE 1	9
.... REFERENCES	16
.... FLOW CHART FOR BASE CASE 1 - FIGURE 2.1	17
.... FLOW TABLE FOR BASE CASE 1 - TABLE 2.1	18
.... TABLE 2.1 CONTINUED	19-23
.... BASE CASE 2	24
.... REFERENCES	30
.... FIGURE 2.2 FLOW CHART FOR BASE CASE 2	31
.... TABLE 2.2 FLOW TABLE FOR BASE CASE 2	32
.... TABLE 2.2 CONTINUED	33-37
.... COMPARISON OF BASE CASES 1 AND 2	38
.... FIGURE 1 PAYBACK PERIOD FOR BASE CASES 1 AND 2	42

APPENDIX 2

.... APPLICATION OF SIMULATED ANNEALING FOR OPTIMIZATION OF CHEMICAL PROCESS FLOWSHEET	43
.... REFERENCES	45

APPENDIX 3

.... ECONOMIC ANALYSIS	46
.... ALCOHOL FUEL AND BY-PRODUCTS MARKETS SUMMARY	47
.... TABLE 2 OXYGENATED BLENDING AGENTS	50
.... TABLE 2 CONTINUED	51

APPENDIX 4

.... I. INSTRUMENTATION	53
.... 1.1 ENGINE	53
.... 1.2 IGNITION SYSTEM	53
.... 1.3 FUEL AIR SYSTEM	54
.... 1.4 LUBRICATION SYSTEM	54
.... 1.5 CYLINDER PRESSURE SYSTEM	55
.... 1.6 DATA PROCESSING SYSTEM	55
.... FIGURE 2 LAYOUT OF INSTRUMENTATION	56
.... 1.7 GAS SAMPLING	57
.... FIGURE 3 SCHEMATIC OF THE BAG SAMPLING & EVACUATION SYSTEM	58
.... FIGURE 4 FORMALDEHYDE AND METHANOL SAMPLING STREAMS	59
.... II. ENGINE TESTS	60

..... TABLE 4 GASOLINE, METHANOL, AND ISOBUTANOL PROPERTIES	62
---	----

..... FIGURE 5 A/F vs. ALCOHOL CONCENTRATION	63
--	----

RESULTS AND DISCUSSION

..... TABLE 5 AIR FUEL RATIO FOR EACH FUEL	64
--	----

..... FIGURE 6 MBT vs. ALCOHOL CONCENTRATION	65
--	----

..... TABLE 6 MBT FOR EACH FUEL	66
---------------------------------------	----

..... REFERENCES	67
------------------------	----

TECHNICAL PROGRESS REPORT

U.S. Department of Energy Contract No. DE-AC22-91PC91034

The Economical Production of Alcohol Fuels
from Coal Derived Synthesis Gas

CONTRACTOR NAME:

West Virginia University Research Corporation
on behalf of West Virginia University
213 Glennlock Hall
Morgantown, WV 26506

Report No.: TPR5

Reporting Period: 10/01/92
to 12/31/92

Due Date: 1/20/93

TASK 1. REACTION STUDIES

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; 2. catalysis research; 1.3 reaction engineering. Research at West Virginia University will be conducted on molybdenum based catalysts. Parallel research will be done at Union Carbide Chemicals and Plastics in South Charleston, WV on metal oxide catalysts. Work at Union Carbide has not yet begun due to problems with contract language. Research at West Virginia University began in July 1992.

The initial focus of this research has been on reaction modeling studies, designing equipment, and developing characterization techniques for molybdenum based catalysts.

1.1 Laboratory Setup

Two computer-controlled, reactor systems have been designed for catalyst testing. One will be a small plug flow reactor for catalyst screening; the second will be a small recirculating autoclave reactor for acquiring engineering data. Each reactor will have four reactant streams for gaseous feeds and one for liquid reactants. The gas feed lines will be for: CO, H₂, H₂S, and an auxiliary line for either He or CO₂/CO. The liquid reactant feed is anticipated to be methanol. Both reactors will have identical front ends for controlling reactant feed rates.

The two reaction units will differ by their reactor design. One will be a small, plug-flow reactor designed to evaluate catalysts of 1

to 10 gram size. This will be appropriate for screening laboratory prepared catalysts. The second will be a small autoclave, with internal mixing, for acquiring engineering data. Analysis of reaction products on both systems will be made with on-line gas chromatographs. Each computer will control one reactor and operate its gas chromatograph for product analysis.

The computers, gas chromatographs, autoclave reactor, furnaces, pumps, flow controllers, and control hardware and software are being ordered to construct these reactor systems. Both will be installed within walkin hoods.

1.2 Catalyst Research

A series of molybdenum, cobalt and molybdenum-cobalt catalysts supported on carbon were prepared by a pore volume impregnation method. Activated carbon with a pore volume of 1.0 ml/g and a total surface area of 660 m²/g was treated with boiling water to remove soluble impurities. Aqueous solutions of (NH₄)₆Mo₇O₂₄ or Co(NO₃)₂ were used for the impregnations. Where two metals were used on the same catalyst, the standard impregnation sequence was molybdenum first followed by cobalt with air drying at room temperature between impregnations. After impregnation, these samples were dried overnight in air at approximately 100 °C. The molybdenum and cobalt sulfides on a carbon support were formed by sulfiding the samples with a 10% H₂S in H₂ mixture, typically at 400 °C for 1 hour. After sulfiding, the samples were purged with helium at 400 °C for 0.5 h, and then cooled in helium to room temperature.

The number of surface anion vacancies, believed to be active sites on metal sulfide catalysts, was counted by using O₂ chemisorption at -78 °C. Measurements were made with a Micromeritics Model 2700 Pulse Chemisorption System. Fresh catalyst samples were sulfided in the chemisorption system, purged with helium and then cooled to measurement temperature.

The effect of order of metal addition on oxygen chemisorption in preparing molybdenum-cobalt catalysts is shown in Table 1. Three catalysts were prepared using hexammonium molybdate and cobalt nitrate solutions. The order of impregnation on the carbon support was varied so that one catalyst had the molybdenum solution added first, was air dried at room temperature, and then the cobalt solution was added. The second had this order reversed. The third catalyst was co-impregnated where both molybdenum and cobalt were added from the same solution. The last catalyst is molybdenum only on the carbon support to provide a point of comparison. All of the samples were sulfided for 1 h. at 400 °C, purged with helium for 0.5 h. at 400 °C, and cooled in helium to adsorption temperature.

Table 1. Effect of Impregnation Order on O₂ Chemisorption with Mo-Co/C Catalysts

Impregnation Order	Composition [wt %]		O ₂ Uptake [μmoles/g]
	Mo	Co	
Mo Added First	4.4	1.6	86.0
Co Added First	4.5	1.6	51.3
Mo,Co Together	4.5	1.6	58.0
Mo Alone	4.5	0.0	48.2

The catalyst prepared by adding the molybdenum solution to the support first had the highest oxygen uptake, suggesting that it had the most catalytic reaction sites. The other procedures produced a catalyst with oxygen chemisorption comparable to that of molybdenum alone on the carbon support. Similar effects of impregnation sequence have been observed for thiophene desulfurization activity with cobalt-molybdenum on carbon catalysts (1). A comparison of oxygen uptake with catalytic performance will be made when the reactor systems are built and operating.

(1) J.C. Duchet, E.M. van Oers, V.H.J. DeBeer and R. Prins. J. Catal. 80, 386 (1983)

1.3 Reactor Engineering

Three computer programs capable of simulating three different types of ideal reactors for higher alcohols synthesis have been developed during this reporting period. These reactors include perfectly mixed batch reactor (PMBR), plug-flow tubular reactor (PFTR), and perfectly mixed continuous stirred tank reactor (CSTR). Listed below are the mathematical models corresponding to each reactor type :

Perfectly Mixed Batch Reactor (PMBR) :

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

Plug Flow Tubular Reactor (PFTR) :

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

Continuous Stirred-Tank Reactor (CSTR) :

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

where N_{j0} , N_j are moles of component j present initially (or in feed) and at any time (or distance) respectively, F_{j0} , F_j are molar flow rate of component j in feed and at any time t respectively, ν_{ij} is the stoichiometric coefficient for species j in the i th reaction, r_i is the rate of reaction in reaction i , W is weight of catalyst, nr is the number of reactions, nc is the number of components, and t is the reaction time for CSTR and PMBR.

The model equations above can also be expressed in terms of conversions as shown below :

$$PMBR : \quad \frac{dX_i}{dt} = \frac{W}{N_{A0}} r_i [p_j(X_i)] ; i = 1, 2, \dots, nr ; j = 1, 2, \dots$$

$$CSTR : \quad \frac{dX_i}{dt} = -X_i + \frac{W}{F_{A0}} r_i [p_j(X_i)] ; i = 1, 2, \dots, nr ; j = 1, 2, \dots$$

$$PFTR : \quad \frac{dX_i}{d\left[\frac{W}{F_{A0}}\right]} = r_i [p_j(X_i)] ; i = 1, 2, \dots, nr ; j = 1, 2, \dots$$

where X_i is the extent of conversion for reaction i , and p_j is the partial pressure of component j .

The system equations described above were solved for the alcohol synthesis reaction model presented in the previous quarterly report using LSODE, a differential equation solver for stiff systems. The three Fortran programs developed are designated as follows: PMBR1 (perfectly mixed batch reactor version 1), CSTR1 (continuous stirred-tank reactor version 1) and PFTR1 (plug-flow tubular reactor version 1). They can be used to calculate moles, mole percent, mole fraction, and partial pressures for each component with time (for CSTR and PMBR) or with position (for PFTR) and the extent of conversion for each reactions. These programs are currently being run on an IBM RISC/6000 and will be available for running on DEC's VAX System in the next reporting period.

Task 1 Coordinator: E. Kugler

TECHNICAL PROGRESS REPORT

U.S. Department of Energy Contract No. DE-AC22-91PC91034

The Economical Production of Alcohol Fuels
from Coal Derived Synthesis Gas

CONTRACTOR NAME:

West Virginia University Research Corporation
on behalf of West Virginia University
213 Glenlock Hall
Morgantown, WV 26506

Report No.: TPR5

Reporting Period: 10/1/92

to 12/31/92

Due Date: 1/20/93

TASK 2. PROCESS SYNTHESIS AND FUEL EVALUATION

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 feed stocks to final product slate.

This report is organized into an executive summary and four appendices which provide more detail on the ideas outlined in the executive summary. The appendices are as follows:

1. Description and Discussion of Base Cases
2. Application of Simulated Annealing for Optimization of Chemical Process Flow Sheets
3. Economic Analysis
4. Fuels Testing

EXECUTIVE SUMMARY

Two base case flow sheets have now been prepared. In the first, which was originally presented in TPR4, a Texaco gasifier is used. Natural gas is also burned in sufficient quantity to increase the hydrogen to carbon monoxide ratio of the synthesis gas to the required value of 1.1 for alcohol synthesis. Acid gas clean up and sulfur removal are accomplished using the Rectisol process followed by the Claus and Beavon processes. About 10% of the synthesis gas is sent to a power generation unit in order to produce electric power, with the remaining 90% used for alcohol synthesis. For this process, the estimated installed cost is \$474.2 MM. The estimated annual operating costs are \$64.5 MM. At a price of alcohol fuels in the vicinity of \$1.00/gal, the pay back period for construction of this plant is about four years. The details of this case, called Base Case 1, are presented in Appendix 1.

The second base case, called Base Case 2, also has a detailed description and explanation in Appendix 1. In Base Case 2, a Lurgi Gasifier is used. The motivation for using a Lurgi Gasifier is that it runs at a lower temperature and pressure and, therefore, produces by-products such as coal liquids which can be sold. Based upon the economics of joint production, discussed in Technical Progress Report 4, this is a necessity. Since synthesis gas from natural gas is always less expensive to produce than from coal, then alcohol fuels will always be less expensive to produce from natural gas than from coal. Therefore, the only way to make coal-derived alcohol fuels economically competitive is to decrease the cost of production of coal-derived synthesis gas. One method for accomplishing this is to sell the by-products from the gasification step. The details of this strategy are discussed in Appendix 3.

Base Case 2 has been prepared so as to produce the same amount of alcohol product as in Base Case 1. Therefore, the same amount of syngas with the same hydrogen to carbon monoxide ratio is produced. Using a Lurgi Gasifier, more coal must be burned placing a higher demand on the oxygen production, acid gas removal and sulfur removal processes. Further, the effluent gas from a Lurgi Gasifier contains a hydrogen to carbon monoxide in excess of 1.1, so pressure swing adsorption is used to remove the excess hydrogen. Steam reforming of natural gas is also not needed. The estimated installed cost of this process is \$771.6 MM, and the estimated annual operating cost is \$113.6 MM/yr. More power and sulfur are produced; and, combined with the large credit taken for selling the coal by-products, the operating credits for non-alcohol products exceed \$100 MM/yr. The pay back period curve for Base Case 2 is very close to that of Base Case 1. At an alcohol price of \$1.00/gal, the pay back period is about 4.5 years.

Now that two different base cases have been developed, each containing different gasifier technology, alternatives within these base cases can be considered. Alternatives to cryogenic oxygen production have already been considered. However, there is strong evidence that cryogenic production is superior to pressure swing adsorption and membrane separations for the volumes needed in these processes. For Base Case 1, alternatives to steam reforming will be investigated. These include sour gas shift conversion, in which carbon monoxide in the acid gas effluent from the gasifier is shifted to form hydrogen and more carbon dioxide, and partial oxidation of natural gas, in which natural gas is partially oxidized into carbon monoxide and hydrogen in an exothermic process, unlike steam reforming which is endothermic. For Base Case 2, it is not clear whether Rectisol and the Claus and Beavon combination are appropriate. With the Lurgi Gasifier operating at lower temperatures and pressures than the Texaco Gasifier more contaminants such as cyanides are present in the acid gas, which makes alternatives to these processes more attractive. These alternatives will be investigated.

In each of the Base Cases, no alcohol purification system has been included. It was assumed that the reactor effluent containing

mixed alcohols and other minor contaminants could be used as an alcohol fuel without further purification. This is probably not true; however, since no product distribution for the alcohols has been determined, there is no purification target. Appendix 3 includes a discussion of the market for different alcohols and Appendix 4 includes a discussion of fuel testing experiments which have begun, ahead of schedule. As the results of these experiments and the market analysis are completed, target alcohol mixtures will be identified and separation schemes will be developed. It is anticipated that the addition of a separation section will not significantly affect the economics of the base cases presented in this report.

Finally, a technique for process optimization is being developed. In complex processes such as this, especially ones which contain discrete choices (i.e., Selexol vs. Rectisol), traditional optimization techniques are not adequate to find a true optimum condition. We will be using the method called simulated annealing, which is ideal for the optimization needed for processes like those involved here. The technique is being developed on a simpler flow sheet first, but will be applied to the base cases as soon as it is ready. The result will be the optimum set of operating temperatures and pressures as well as the optimum set of choices of alternative units within the process. This method is described in Appendix 2.

Task 2 Coordinator: J. Shaeiwitz

Appendix 1

Base Case 1

rev 12/29/92

The following report gives a brief description of each of the units in the block flow diagram. 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 (1) (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.

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) = \$15.1 MM

COAL PREPARATION

Coal (stream 10), limestone (stream 11), and water (stream 12), are sent to the Coal Preparation Block. Limestone is added for sulfur reduction. 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 = 1.5 MW

Installed Capital Cost (1992 dollars) = \$41.1 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 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 = 1300 lbs/hr 250 psig, 530° F

Installed Capital Cost (1992 dollars) = \$66.1 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 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 = 0.8 MW

Steam needs = 2500 lbs/hr saturated 100 psig

18000 lbs/hr 50 psig at 300° F

Installed Capital Cost (1992 dollars) = \$32.9 MM

TEXACO GASIFIER

The coal slurry (stream 13) is mixed with compressed oxygen (stream 9) and burned at 2300—2800°F and 1180 psig 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 = 0.4 MW

Steam needs = 9100 lbs/hr 50 psig, 300° F

Installed Capital Cost (1992 dollars) = \$141.1 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) = \$2.6 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 2300° F and 1180 psig enters the Syngas Heat Recovery Block and is cooled against process boiler feed water at 60° F (stream 71). The raw gas stream exits at 630° F (stream 18), and the boiler feed exits as steam at 1500 psig and 900°F (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 = 3.36×10^8 Btu/hr

Power needs = 0.3 MW

Installed Capital Cost (1992 dollars) = \$6.7 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 = 10000 lbs/hr saturated 700 psig
7500 lbs/hr 250 psig at 530° F

Installed Capital Cost (1992 dollars) = \$9.6 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) = \$3.6 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 (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 1500 psig, 900°F 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 slightly above 50 MW. Therefore, it is assumed that the cost for these blocks will be roughly equivalent to Houston plant 31.

Power produced = 54.6 MW

Installed Capital Cost (1992 dollars) = \$65.8 MM

STAND ALONE COMPRESSORS AND POWER SUMMARY

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 (5).

FUNCTION	INLET STREAM	P (atm)	OUTLET STREAM	P (atm)	POWER (MW)	COST (MM\$)
Air Prep	—	1	1	5	-24.0	0.7
O ₂ Prep	2	1	9	80	- 8.8	14.7
CH ₄ Prep	—	2	14	80	- 2.4	5.1
Rxtr Prep	22	80	26	140	- 5.2	9.7
Recy Comp	56A	125	56B	140	- 0.7	2.0
Total compressor needs					-41.1	
Other in plant needs					- 6.6	
Total produced in steam and gas turbines					+54.6	
Net power output					+ 6.9	
Total installed compressor costs (1992 dollars)						32.2

TOTAL ESTIMATED CAPITAL INVESTMENT (MM\$)

Synthesis Gas via Methane	15.1
Coal Preparation	41.1
Texaco Gasifier	141.1
Slag Handling	2.6
Steam/Power Generation	65.8
Synthesis Gas Heat Recovery	6.7
Cryogenic Oxygen Production	66.1
Rectisol (Acid Gas Separation)	32.9
COS Hydrolysis	
Claus (Sulfur Recovery)	9.6
Beavon	3.6
MoS ₂ Alcohol Synthesis Loop	40.0
CO ₂ Removal in Alcohol Synthesis Loop	15.6
Other Compressors	32.2
TOTAL	472.4

OVERALL ECONOMIC EVALUATION

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\$)		472.4
TOTAL ESTIMATED OPERATING COSTS (MM\$/YR)		64.5
Coal (\$30/ton delivered)	21.2	
Natural Gas (\$3/MSCF)	11.3	
Other Expenses	32.0	
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS) (MM\$/YR)		8.7
Power (\$0.05/kW-hr)	2.8	
Slag (\$5/ton) (6)	0.4	
Sulfur (\$13.60/100 lbs.) (7)	5.5	

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.

IMPORTANT POINTS OF INFORMATION

Several decisions were made for the creation of this base case which should be outlined. Also, there are alternatives which have not been fully considered which will be considered in more detail later. They are listed below along with the reasons behind them.

- Catalytic steam/methane reformation used to adjust the $H_2:CO$ ratio upwards. The ratio from coal gasification is less than 1. Since the optimal ratio for higher alcohol synthesis is approximately 1.2, an additional source of hydrogen was required. The reformer was assumed to operate at equilibrium, as suggested in the literature (8). Other alternatives to this block are available and will be considered.
- The traditional method for purifying high quantities of pure oxygen is by cryogenics, which is used for the base case. However, recent reports suggest that membrane and catalytic processes are becoming economically competitive with cryogenics. Therefore, we will examine these alternatives, especially since oxygen production is the second most costly block in the base case.
- The Rectisol system was chosen as the base case system for H_2S and COS removal. The major alternative to Rectisol is Selexol. The literature indicates that Rectisol has a higher installed capital cost, but a lower fixed operating cost than Selexol. Both of these systems are capable of removing H_2S to the ppm level and beyond. However, there is some evidence that quantities of H_2S are beneficial if the reaction involves the MoS_2 catalyst. If this is so, then a system such as the Benfield acid gas removal process might be more suitable. The Benfield system does not remove as much H_2S and has lower capital and operating costs.
- The operating pressure for the Texaco gasifiers has been set at 80 atmospheres. This is the highest pressure indicated in the literature at which a Texaco gasifier has been run. Since the pressure required at the reactor is 140 atmospheres, we would of course like to run the gasifiers at as high a pressure as possible. Another limiting factor is the oxygen feed pressure. According to various sources, the highest pressure available with conventional centrifugal compressors is around 60 atmospheres. It is assumed that, because of the size of the base case, a higher cost for the oxygen compressor would be acceptable in return for savings on feed gas compression. In addition, other gasification systems will also be investigated.
- As a place to start, approximately 7% of the total clean syngas is diverted for steam generation and power production, resulting in an overall net power surplus of approximately 7 MW. Factors such as the demand for mixed alcohols or the price of electricity will be considered in order to determine suitable splits.

REFERENCES

1. *Final Report on the Houston Area Medium-BTU Coal Gasification Project, Volumes 2 and 3.* Prepared by the Linde Division of Union Carbide Corporation, June 1982.
2. Baasel, William D., *Preliminary Chemical Engineering Plant Design*, 2nd edition, Van Nostrand Reinhold, New York, 1990, pp.268-269.
3. "Beavon Sulfur Removal Process," *Hydrocarbon Processing*, April 1984.
4. Frank, Marshall E. "Methanol: Emerging Uses, New Synthesis," *Chemtech*, June 1982.
5. Baasel, pp.529-530.
6. T. Torries, personal communication
7. *Chemical Marketing Reporter*, August 31, 1992.
8. Rase, Howard F., *Chemical Reactor Design for Process Plants, Volume 2*, John Wiley & Sons, New York, 1977, pp.133-138.

BASE CASE #1

Rev 1 7/2/82 Rev 2 8/5/82 Rev 3 8/10/82 Rev 4 12/7/82

FLOW CHART FOR BASE CASE 1 - FIGURE 2.1

Base Case 1	001	001A	002	003	004	006	008	009	010	011
Ar	94.1	94.1	0.0	0.0	0.0	94.1	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	4474.2	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	21.2	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
CO	0.0	0.0	0.0	0.0	0.0	0.0	3269.0	0.0	0.0	0.0
CO2	3.3	3.3	0.0	0.0	0.0	0.0	1181.2	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	2.8	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	3.7
H2	0.0	0.0	0.0	0.0	0.0	0.0	2410.2	0.0	1828.3	0.0
H2O	243.3	243.3	0.0	0.0	0.0	0.0	3100.0	0.0	51.5	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	57.3	0.0	0.0	0.0
N2	7882.0	7882.0	0.0	7882.0	7161.4	0.0	36.3	0.0	39.6	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	6.6	0.0	0.0	0.0
O2	2119.0	2119.0	2119.0	0.0	0.0	0.0	0.0	2119.0	352.4	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	60.1	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	83.8	0.0
kmol/hr	10341.7	10341.7	2119.0	7882.0	7161.4	94.1	10084.6	2119.0	6889.9	3.7
kg/hr	296792.1	296792.1	67808.0	220695.7	200518.9	3763.2	207541.2	67808.0	81130.8	370.0
Temp. (C)	262.0	25.0	25.0	25.0	25.0	25.0	1300.0	40.0	25.0	25.0
Press. (psi)	75.0	15.0	30.0	30.0	30.0	30.0	1180.0	1180.0	15.0	15.0

	012	013	014	14A	015	017	017A	018	019	020
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	4474.2	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	18.0
CH4	0.0	0.0	595.2	595.2	0.0	4.8	0.0	21.2	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
CO	0.0	0.0	0.0	0.0	0.0	194.9	0.0	3269.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	395.4	0.0	1181.2	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.8	0.0	0.0
CaCO3	0.0	3.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	1828.3	0.0	0.0	0.0	2166.6	0.0	2410.2	0.0	0.0
H2O	3740.0	3791.5	0.0	0.0	7907.5	6921.7	10021.7	3100.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	57.3	0.0	0.0
N2	0.0	39.6	0.0	0.0	0.0	0.0	0.0	36.3	720.6	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.6	0.0	0.0
O2	0.0	352.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	60.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	83.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	3740.0	10633.6	595.2	595.2	7907.5	9683.4	10021.7	10084.6	720.6	18.0
kg/hr	67320.0	148820.8	9523.2	9523.2	142335.0	151855.5	180390.6	207541.2	20176.8	576.0
Temp. (C)	25.0	25.0	135.0	25.0	300.0	25.0	25.0	25.0	25.0	25.0
Press. (p	15.0	1180.0	1180.0	29.0	1180.0	1180.0	1180.0	1180.0	30.0	15.0

	022	022A	023	024	025	026	026A	027	028	033
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	18.0	0.0	319.8	0.0	0.0	0.0
CH4	26.0	25.8	0.0	0.0	0.0	25.8	257.4	25.7	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	695.5	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	250.7	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	93.8	0.0	0.0	0.0
CO	3463.9	3429.3	0.0	0.0	0.0	3429.3	2860.9	286.1	0.0	0.0
CO2	0.0	0.0	946.0	551.8	78.8	0.0	247.8	34.8	3.3	0.0
COS	0.0	0.0	0.0	0.0	2.8	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	3.7
H2	4576.8	4531.0	0.0	0.0	0.0	4531.1	3426.8	342.7	0.0	0.0
H2O	0.0	0.0	0.0	0.0	0.0	0.0	41.9	0.0	243.3	0.0
H2S	0.0	0.0	0.0	0.0	57.3	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	756.9	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	6.6	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	0.0	0.0	0.0	83.8
kmol/hr	8066.7	7986.1	946.0	1308.7	163.5	7986.1	8184.6	689.3	246.6	87.5
kg/hr	106558.9	105495.2	41624.0	45472.4	6103.6	105493.6	166204.4	10638.6	4523.9	8919.6
Temp. (C)	25.0	25.0	25.0	25.0	25.0	310.0	310.0	50.0	25.0	1300.0
Press. (p	1180.0	1180.0	15.0	15.0	15.0	2060.0	2060.0	2060.0	30.0	1180.0

	034	036	037	038	039	041	042	045	046	047	048
Ar	0.0	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	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	18.0	0.0	18.0	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.3	0.0	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	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	0.0
C4H10O	0.0	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	34.6	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	78.8	0.0	78.8	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	0.0
CaCO3	0.0	0.0	3.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	45.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	200.0	200.0	0.0	0.0	0.0	0.0	0.0	51.6	0.0	0.0	20.0
H2S	0.0	0.0	0.0	0.0	0.0	69.1	0.0	5.7	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	89.2	0.0	89.2	89.2	0.0	12.8	0.0
NH3	0.0	0.0	0.0	0.0	0.0	6.6	0.0	6.6	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	32.0	0.0	32.0	6.2	0.0	3.4	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	51.6	0.0	0.0
Al2O3	0.0	0.0	83.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	200.0	200.0	87.5	80.6	121.2	163.5	121.2	256.1	51.6	16.2	20.0
kg/hr	3600.0	3600.0	8919.6	1065.4	3520.4	6198.8	3520.4	7974.0	1651.2	466.9	360.0
Temp. (C)	25.0	156.0	156.0	25.0	25.0	25.0	25.0	370.0	370.0	25.0	25.0
Press. (p	500.0	15.0	15.0	1180.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0

	050	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	0.0
C	0.0	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	0.0	0.0	0.0	0.0	319.8	0.0
CH4	0.0	0.0	0.0	231.6	231.9	231.9	0.0	257.4	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	695.5	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	250.7	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	83.8	0.0
CO	0.0	0.0	0.0	2574.7	2645.3	2574.7	0.0	2860.8	0.0	0.0	0.0
CO2	78.8	0.0	0.0	313.0	0.0	0.0	313.0	247.8	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	0.0
CaCO3	0.0	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	3084.1	3076.4	3084.1	0.0	3426.8	0.0	0.0	0.0
H2O	0.0	0.0	57.3	0.0	0.0	0.0	0.0	0.0	41.9	0.0	241.6
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	102.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	6.6	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	0.0
S	0.0	5.7	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	0.0
kmol/hr	205.4	5.7	57.3	6203.4	5953.6	5890.7	313.0	6792.8	41.9	1349.8	241.6
kg/hr	7011.4	183.4	1031.4	95737.4	83931.6	81970.2	13772.0	101977.6	754.2	63469.8	4348.8
Temp. (C)	370.0	25.0	370.0	310.0	310.0	310.0	25.0	310.0	25.0	25.0	25.0
Press. (p	15.0	15.0	15.0	1840.0	1840.0	2060.0	15.0	1840.0	15.0	15.0	15.0

	067	068	070	071	073	074	075
Ar	17.7	0.0	0.0	0.0	0.0	0.0	17.7
C	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
CH4	0.0	0.0	25.7	0.0	0.0	0.0	0.0
C2H6O	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
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	286.1	0.0	0.0	0.0	0.0
CO2	0.0	0.0	34.8	0.0	0.0	0.0	346.6
COS	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
H2	0.0	0.0	342.7	0.0	0.0	0.0	0.0
H2O	0.0	6104.0	0.0	6104.0	2611.3	2611.3	635.8
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	1380.6	0.0	0.0	0.0	0.0	0.0	1380.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	369.5	0.0	0.0	0.0	0.0	0.0	16.5
S	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
kmol/hr	1767.7	6104.0	689.3	6104.0	2611.3	2611.3	2397.2
kg/hr	51186.6	109871.6	10638.6	109872.0	47003.4	47003.4	66587.0
Temp. (C)	25.0	482.0	25.0	20.0	20.0	482.2	25.0
Press. (P)	15.0	1514.0	15.0	1515.0	1515.0	1515.0	15.0

The following report gives a brief description of each of the units in the block nOw diagram. 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 (1) (All references to material in this report will be referred to as Houston). 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.

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 do 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 = 3.8 MW

Installed Capital Cost (1992 dollars) = \$75.2 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 = 2100 lbs/hr 250 psig, 530° F

Installed Capital Cost (1992 dollars) = \$114.4 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 = 4.4 MW

Steam needs = 14000 lbs/hr saturated 100 psig

100000 lbs/hr 50 psig at 300° F

Installed Capital Cost (1992 dollars) = \$99.7 MM

LURGI GASIFIER

The coal slurry (stream 13) is mixed with compressed oxygen (stream 9) and burned at 900°F and 1180 psig 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 .

Power needs = 1.0

Steam needs = 23000 lbs/hr 50 psig, 300° F

Installed Capital Cost (1992 dollars) = 220.6 MM\$

SLAG HANDLING

Molten slag from the Lurgi 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) = 4.8 \$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.

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 = 0.5
Steam needs = 25000 lbs/hr saturated 700 psig
18000 lbs/hr 250 psig at 530° F
Installed Capital Cost (1992 dollars) = \$17.6 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) = \$6.6 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

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 1500 psig, 900° F 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 150 MW. Therefore, it is assumed that the cost for these blocks can be exponentially scaled from Houston plant 31.

Power needs = 160.0 MW

Installed Capital Cost (1992 dollars) = \$134.4 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

STAND ALONE COMPRESSORS AND POWER SUMMARY

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 (4).

FUNCTION	INLET STREAM	P (atm)	OUTLET STREAM	P (atm)	POWER (MW)	COST (MM\$)
Air Prep	—	1	1	5	— 38.4	1.0
O ₂ Prep	2	1	9	80	— 14.1	20.0
Rxtr Prep	22	80	26	140	— 5.2	9.7
Recy Comp	56A	125	56B	140	— 0.7	2.0
Total compressor needs					— 58.4	
Other inplant needs					— 9.8	
Total produced in steam and gas turbines					160.0	
Net power output					91.8	
Total installed compressor costs (1992 dollars)						32.7

TOTAL ESTIMATED CAPITAL INVESTMENT (MM\$)

Coal Preparation	75.2
Lurgi Gasifier	220.6
Slag Handling	4.8
Steam/Power Generation	134.4
Cryogenic Oxygen Production	114.4
Rectisol (Acid Gas Separation)	99.7
COS Hydrolysis	
Claus (Sulfur Recovery)	17.6
Beavon	6.6
MoS ₂ Alcohol Synthesis Loop	40.0
CO ₂ Removal in Alcohol Synthesis Loop	15.6
Other Compressors	32.7
Pressure Swing Adsorption	10.0
TOTAL	771.6

OVERALL ECONOMIC EVALUATION

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\$)	771.6
TOTAL ESTIMATED OPERATING COSTS(MM\$/YR)	113.6
Coal (\$30/ton delivered)	53.6
Other Expenses	60.0
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS) (MM\$/YR)	110.2
Power (\$0.05/KW-hr)	37.3
Slag (\$5/ton) (5)	1.0
Sulfur (\$13.60/100 lbs.) (6)	13.9
Coal Tar/Liquid By-Products	58.0

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

IMPORTANT POINTS OF INFORMATION

Several decisions were made for the creation of this base case which should be pointed out. Also, there are alternatives which have not been fully considered which should be viewed in more detail. They are listed below along with the reasons behind them.

- The traditional method of producing large quantities of pure oxygen is by cryogenics, which is used for the base case. However, recent reports have suggested that membrane and catalytic processes are becoming economically competitive with cryogenics. Therefore, we suggest that more research be done in this area, especially since it is the second most costly block in the base case.
- The Rectisol system was chosen as the base case system for H_2S and COS removal. The major alternative to Rectisol is Selexol. The literature indicates that Rectisol has a higher installed capital cost, but a lower fixed operating cost than Selexol. Both of these systems are capable of removing H_2S to the ppm level and beyond. However, there is some evidence that substantial quantities of H_2S are beneficial in the reaction stages of the base case. If this is so, then a system such as the Benfield Acid Gas removal process might be more suitable. The Benfield system does not remove as much H_2S and has lower capital and operating costs.
- The operating pressure for the Lurgi Gasifiers has been set at 80 atmospheres. No data has been found on the maximum pressure that a Lurgi Gasifier can be run. Since the pressure required at the reactor is 140 atmospheres, we would of course like to run the gasifiers at as high a pressure as possible. Another limiting factor is the oxygen feed pressure. According to various sources, the highest pressure available with conventional centrifugal devices is around 60 atmospheres. It is assumed that, because of the size of the base case, a higher cost for the oxygen compressor would be acceptable in return for savings on feed gas compression. In addition to these concerns, there are other gasification systems which should be investigated.
- As a place to start, approximately 7 percent of the total clean syngas is diverted for steam generation and power production. This resulted in an overall net power surplus of approximately 92 MW. Factors such as the demand for mixed alcohols or the price of electricity should be considered for deciding on what splits should be studied.

REFERENCES

1. *Final Report on the Houston Area Medium-BTU Coal Gasification Project, Volumes 2 and 3.* Prepared by the Linde Division of Union Carbide Corporation, June 1982.
2. "Beavon Sulfur Removal Process," *Hydrocarbon Processing*, April 1984.
3. Frank, Marshall E. "Methanol: Emerging Uses, New Synthesis," *Chemtech*, June 1982.
4. Baasel, pp.529-530.
5. T. Torries, personal communication
6. *Chemical Marketing Reporter*, August 31, 1992.

BASE CASE #2

FIGURE 2.2 FLOW CHART FOR BASE CASE 2

Base Case 2	001	001A	002	003	004	006	008	009	010	011
Ar	150.6	150.6	0.0	0.0	0.0	150.6	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	11435.0	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	1748.9	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
C3H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10	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	3429.3	0.0	0.0	0.0
CO2	5.3	5.3	0.0	0.0	0.0	0.0	4693.8	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	6.2	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	10.5
H2	0.0	0.0	0.0	0.0	0.0	0.0	8163.6	0.0	4672.8	0.0
H2O	389.3	389.3	0.0	0.0	0.0	0.0	14400.0	0.0	131.6	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	147.4	0.0	0.0	0.0
N2	12611.0	12611.0	0.0	12611.0	7161.4	0.0	91.9	0.0	101.2	0.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	18.7	0.0	0.0	0.0
O2	3390.4	3390.4	3390.4	0.0	0.0	0.0	0.0	3390.4	900.7	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	153.6	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	214.2	0.0
kmol/hr	16546.6	16546.6	3390.4	12611.0	7161.4	150.6	32699.9	3390.4	17609.1	10.5
kg/hr	474864.5	474865.4	108492.8	353108.0	200519.2	6024.0	613964.3	108492.8	207354.0	1050.0
Temp. (C)	262.0	25.0	25.0	25.0	25.0	25.0	1300.0	40.0	25.0	25.0
Press. (psi)	75.0	15.0	30.0	30.0	30.0	30.0	1180.0	1180.0	15.0	15.0

	012	013	017A	018	019	020	022	022A	022AA	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	11435.0	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
CH4	0.0	0.0	0.0	1748.9	0.0	0.0	1748.9	1731.5	1731.5	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
CO	0.0	0.0	0.0	3429.3	0.0	0.0	3429.3	3395.0	3395.0	0.0
CO2	0.0	0.0	0.0	4693.9	0.0	0.0	0.0	0.0	0.0	2816.3
COS	0.0	0.0	0.0	6.2	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	10.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	4672.8	0.0	8163.6	0.0	0.0	8163.6	4531.0	0.0	0.0
H2O	19700.0	19831.6	14400.0	14400.0	0.0	0.0	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	147.4	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	101.2	0.0	91.9	5449.8	0.0	0.0	0.0	8082.0	0.0
NH3	0.0	0.0	0.0	18.7	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	900.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	153.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	214.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	19700.0	37319.6	14400.0	32699.9	5449.8	18.0	13341.8	9657.5	13208.5	2816.3
kg/hr	354600.0	563004.0	259200.0	613964.3	152594.4	576.0	140330.0	131826.0	349060.0	123917.2
Temp. (C)	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0
Press. (p)	15.0	1180.0	1180.0	1180.0	30.0	15.0	1180.0	1180.0	1190.0	15.0

	024	025	026	026A	027	027A	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	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1557.0	0.0	0.0	1557.0
CH3OH	0.0	18.0	0.0	319.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	1731.4	17305.0	1730.4	0.0	0.0	0.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	695.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	250.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	83.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	3395.0	2518.5	251.9	0.0	0.0	0.0	0.0	0.0	0.0
CO2	1642.8	234.7	0.0	347.8	34.8	0.0	5.3	0.0	0.0	0.0	0.0
COS	0.0	6.2	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	10.5	0.0	0.0	10.5
H2	0.0	0.0	4531.0	3426.8	342.7	3551.0	0.0	1672.1	0.0	0.0	1672.1
H2O	0.0	0.0	0.0	41.9	0.0	0.0	389.3	0.0	200.0	200.0	0.0
H2S	0.0	147.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	5541.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	18.7	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	787.4	0.0	0.0	787.4
S	0.0	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	214.2	0.0	0.0	214.2
kmol/hr	7184.5	425.0	9657.4	24989.8	2359.8	3551.0	394.6	4241.2	200.0	200.0	4241.2
kg/hr	227449.4	16232.3	131824.4	433778.8	36956.2	7102.0	7240.6	70123.4	3500.0	3600.0	70123.4
Temp. (C)	25.0	25.0	310.0	310.0	50.0	25.0	25.0	1300.0	25.0	156.0	156.0
Press. (p	15.0	15.0	2060.0	2060.0	2060.0	1180.0	30.0	1180.0	500.0	15.0	15.0

	038	039	041	042	045	046	047	048	050	051	054
Ar	0.0	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	0.0
CH3OH	0.0	0.0	18.0	0.0	18.0	0.0	0.0	0.0	18.0	0.0	0.0
CH4	17.5	0.0	0.0	0.0	0.0	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	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	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	34.3	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	234.7	0.0	234.7	0.0	0.0	0.0	234.7	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	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	81.6	0.0	0.0	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	132.7	0.0	0.0	20.0	0.0	0.0	147.4
H2S	0.0	0.0	153.6	0.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	89.2	0.0	254.2	254.2	0.0	36.5	0.0	290.7	0.0	0.0
NH3	0.0	0.0	18.7	0.0	18.7	0.0	0.0	0.0	18.7	0.0	0.0
O2	0.0	32.0	0.0	91.2	24.9	0.0	9.7	0.0	27.2	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	132.7	0.0	0.0	0.0	14.8	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
kmol/hr	133.4	121.2	425.0	345.4	698.2	132.7	46.2	20.0	589.3	14.8	147.4
kg/hr	1403.6	3520.4	16443.1	10036.0	22033.7	4246.4	1332.4	360.0	20230.7	473.6	2653.2
Temp. (C)	25.0	25.0	25.0	25.0	370.0	370.0	25.0	25.0	370.0	25.0	370.0
Press. (p	1180.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0

	056	056A	056B	057	059	063	064	065	067	068
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	150.5	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	319.8	0.0	0.0	0.0
CH4	15574.0	15574.0	15574.0	0.0	17304.0	0.0	0.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	695.5	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	250.7	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	83.8	0.0	0.0	0.0
CO	2266.7	2266.7	2266.7	0.0	2518.6	0.0	0.0	0.0	0.0	0.0
CO2	313.0	0.0	0.0	313.0	347.8	0.0	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	3084.1	3084.1	3084.1	0.0	3426.8	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	0.0	0.0	41.9	0.0	241.6	0.0	6104.0
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	11735.0	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	3140.8	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
kmol/hr	21237.8	20924.8	20924.8	313.0	23597.2	41.9	1349.8	241.6	15026.3	6104.0
kg/hr	332591.8	318819.8	318819.8	13772.0	369541.6	754.2	63469.8	4348.8	435105.6	109871.6
Temp. (°C)	310.0	310.0	310.0	25.0	310.0	25.0	25.0	25.0	25.0	482.0
Press. (p	1840.0	1840.0	2060.0	15.0	1840.0	15.0	15.0	15.0	15.0	1514.0

TABLE 2.2 (CONTINUED)

	070	071	073	074	075
Ar	0.0	0.0	0.0	0.0	150.5
C	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0
CH4	1730.4	0.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0
CO	251.9	0.0	0.0	0.0	0.0
CO2	34.8	0.0	0.0	0.0	2017.1
COS	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0
H2	342.7	0.0	0.0	0.0	0.0
H2O	0.0	6104.0	23502.0	23502.0	4045.1
H2S	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	11735.0
NH3	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	247.9
S	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0
kmol/hr	2359.8	6104.0	23502.0	23502.0	18195.6
kg/hr	36956.2	109872.0	423036.0	423036.0	504097.0
Temp. (C)	25.0	20.0	20.0	482.2	25.0
Press. (P	15.0	1515.0	1515.0	1515.0	15.0

TABLE 2.2 (CONTINUED)

Comparison of Base Cases 1 and 2

The goal of Base Case 2 is to compare the Texaco Gasification system with the Lurgi Gasification system. To that end, all features of Base Case 1 were incorporated into Base Case 2 with two exceptions. The ratio of H_2 to CO in the syngas sent to the reactor must be approximately 1.1. From the Texaco gasifiers, this ratio is less than 1, so additional hydrogen is supplied by the steam reformation of natural gas. From the Lurgi gasifiers, this ratio is almost 2, so hydrogen is removed via a Pressure Swing Adsorption block, and the steam reformation block has been removed. The constraint placed on the comparison is that the same quantity of mixed alcohols (170 MM gal) is produced in each case. All flowrates from Base Case 1 are adjusted to meet this specification. A comparison of the payback period for each base case plant versus the price of the alcohol fuel product is presented in the attached figure.

Lurgi Gasification versus Texaco Gasification

Where as the Texaco gasifier operates at very high temperatures (1300 – 1500°C), the Lurgi gasifier operates at comparatively mild temperatures (400 – 500°C). Two major consequences result from this and other operating differences between the gasifiers. First, as stated above, the ratio of H_2 to CO in the syngas is much higher than desired for the downstream reactions. A larger percentage of the carbon in the coal is converted to methane in the Lurgi than in the Texaco. Second, the low temperatures cause an incomplete gasification of the coal volatiles. Coal tars, coke, phenolic compounds, and other by-products are produced from these ungasified volatiles. These by-products are fairly valuable and can be purified and sold. However, in order to produce the same quantity of mixed alcohols taking the above into account, the coal feed rate to the gasifiers must be increased by 153%. This causes the gasifier installation costs as well as other major block installation costs to increase by almost 100%, and the raw material costs increase by a factor of 153%. The advantage of the Lurgi is the increase in non-alcohol related plant credits. The by-products mentioned above are valued at approximately \$58 MM. Also, the large amount of methane produced in the gasifier can be combusted and the heat produced can be used to raise high pressure steam, which in turn can be used to generate electricity. The resulting power credits amount to \$37 MM. Three tables are presented below which compare the economics of the two base cases.

	Operating Costs (MM\$/YR)	
Coal	21.2	53.6
Natural Gas	11.3	0.0
Other Expenses	32.0	60.0
Total	64.5	113.6

	Installed Costs (MM\$)	
	Texaco	Lurgi
Syngas via Methane	15.1	0.0
Pressure Swing Adsorption	0.0	10.0
Coal Preparation	41.1	75.2
Gasifier	141.1	220.6
Slag Handling	2.6	4.8
Steam/Power Generation	65.8	134.4
Syngas Heat Recovery	6.7	0.0
Cryogenic Oxygen Production	66.1	114.4
Rectisol	32.9	99.7
Claus and Beavon	13.2	24.2
Alcohol Synthesis	40.0	40.0
CO ₂ Removal	15.6	15.6
Compressors	32.2	32.7
Total	472.4	771.6

	Operating Credits (excluding alcohols) (MM\$/YR)	
Power	2.8	37.3
Slag	0.4	1.0
Sulfur	5.5	13.9
By-Products	0.0	58.0
Total	8.7	110.2

Some of the changes required to use the Lurgi gasifier as opposed to the Texaco gasifier are summarized below.

Coal Feed Rate and Gasifier Economics

From the Base Case 1 flowsheet, the above goal is fulfilled when stream 26 is the same for both Base Cases. The basis for the coal feed rate then is the flow of CO, since this is the limiting coal product. Stream 26 contains 3429.3 kmol/hr of CO. The raw gas output from the Lurgi Gasifier contains 7.99 kmol of CO per 465 kg of dry, ash free coal. Calculations indicate that 205,000 kg/hr of coal would be required to meet stream 26 requirements. This is 2.53 times more than base case 1. The main reason for this large increase is the reversal in the $H_2:CO$ ratio.

Cryogenic Oxygen Plant

The Texaco Gasifier requires a 1 to 1 mass ratio of oxygen to coal, while for the Lurgi Gasifier the ratio is 0.55 to 1. Combining this factor with the increased coal usage, the amount of oxygen required is about 1.6 times that for Base Case 1.

Rectisol

The raw gas stream entering rectisol contains about 5.5 times as much carbon dioxide as does the stream in Base Case 1. This number was used in an exponential function to determine the new capital cost.

Pressure Swing Adsorption

This unit must be added to the flowsheet to remove the excess hydrogen from the pre-reactor stream. From the Houston report used for cost data in Base Case 1, the cost of a PSA unit is \$14MM (1981). Although the rationale behind costing this unit is unknown, it should be cheaper than this value for at least two reasons. First, the total feed rate is 25% less than the Houston plant. Second, the recovery of hydrogen desired is only 50% whereas the recovery in the Houston report is 87%. In addition, hydrogen purity may not be essential because it will be used as fuel unless a market is found.

Stand Alone Compressors

The Reactor Prep and Recycle compressors are exactly the same as before. The Air Prep compressor is 1.6 times bigger as is the O_2 prep compressor. The CH_4 prep compressor has been eliminated.

Power Summary

2.53 times as much coal is used, but its outlet temperature is much lower and cannot be used to raise high pressure steam. However, the large amount of methane generated can be sent to the combustion unit in power generation, and the heat of reaction can be used to generate steam. The end result is that 3 times as much electricity is generated in Base Case 2 (Lurgi) than in Base Case 1 (Texaco). Note that if no market can be found for the excess hydrogen that is removed in the pressure swing adsorption block, it could be used as a fuel also to generate more electricity.

FIGURE 1

Appendix # 2

Application of Simulated Annealing for Optimization of Chemical Process Flowsheet

Simulated annealing is an algorithm for single objective multi-variable optimization problems and is based on the Monte-Carlo method for the simulation of physical systems (Metropolis, et al., 1953). Simulated annealing draws an analogy between the minimization of energy achieved by annealing a physical system and the minimization of a cost function required in optimization (Kirkpatrick, et al., 1983). Simulated annealing asymptotically converges to a global optimal solution to every combinatorial optimization problem under the limiting condition of infinite computation time. However, in realistic situations, it is the finite time behavior or the use of simulated annealing as an approximate algorithm which is of greater interest. As an approximate algorithm, simulated annealing provides near-optimal solutions in polynomial time to exponential time problems (Aarts and van Laarhoven, 1985).

The algorithm for simulated annealing consists of repeatedly making a move to change the system configuration and accepting or rejecting the move based on a mathematically derived acceptance probability, while periodically reducing the annealing temperature. The algorithm is made to terminate when a specified termination criterion is satisfied. The annealing schedule and the move acceptance criterion used in this work are the Aarts and van Laarhoven annealing schedule (Aarts and van Laarhoven, 1985) and the Metropolis move acceptance criterion (Metropolis, et al., 1953). The Aarts and van Laarhoven schedule reduces the annealing temperature by using a multiplicative factor that depends on the proximity to equilibrium reached at the present temperature. It should be noted that the multiplicative factor is less than 1. The Metropolis move acceptance criterion accepts a decreasing number of moves as the temperature is lowered. All moves that lead to an improvement in the objective function are accepted, while moves that tend to deteriorate the objective function are

accepted with a probability that depends on the deterioration and the annealing temperature. The higher the deterioration and the lower the annealing temperature, the lower is the probability of the move being accepted. Thus, as the annealing temperature decreases, the objective function improves and reaches the global optimum under the limiting condition of infinite moves. This move acceptance criterion allows simulated annealing to climb out of local minima and this differentiates the algorithm from greedy search algorithms which accept only downhill moves.

The optimization of a process flowsheet can be treated as a single objective optimization problem with a large number of variables. The total installed and operating cost of the chemical plant can be considered as the single objective with respect to which the optimization is done. The operating conditions such as pressure, temperature, flowrates, etc. can be considered as the variables which affect the cost of the plant. Constraints can be incorporated for the plant to operate in a flexible and feasible manner to manufacture the products from the raw materials.

As a chemical plant would consist of a very large number of pieces of equipment, the problem is very complex and difficult to solve. Additionally, it is very inefficient to compute a new cost for each process due to changes in a processing variable upstream. Initially, as a simplification, the cost of each piece of equipment is calculated over a wide range of processing conditions and flowrates; and, the data generated is regressed over a polynomial equation. Using the equations generated, an approximate cost can be computed with limited computational effort for each piece of equipment when there is a change in a variable upstream or in the equipment itself. Thus, the overall cost of the plant can be approximated within an acceptable range. Each variable can be manipulated within a certain range and only feasible solution space is considered. The costing of the various pieces of equipment is done by using Aspen Plus.

References

Aarts E.H.L. and P.J.M. van Laarhoven. Statistical Cooling: A General Approach to Combinatorial Optimization Problem, *Phillips Journal of Research*, **40**, 193, (1985).

Kirkpatrick S., C.D. Gelatt Jr., and M.P. Vecchi. *Optimization by Simulated Annealing*, *Science*, **220**, 671, (1983)

Metropolis N., A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, and E. Teller. Equation of State Calculations by Fast Computing Machines, *Journal of Chemical Physics*, **21**, 1087, (1953).

Appendix 3

Economic Analysis

Spreadsheet Model

The alcohol production process has been divided into two stages. The first stage entails those steps required to produce synthesis gas while the second stage deals with the steps involved with the transformation of the synthesis gas into the alcohol fuel and waste. Since the alcohol product can be manufactured from synthesis gas derived from either coal or natural gas, the price of the synthesis gas derived from its respective source becomes a critical factor in determining the choice of feed stock. If coal is to be used as the primary feed stock, then the cost of coal derived synthesis gas (syngas) must be lower than synthesis gas derived from natural gas.

Preliminary investigations, however, suggest that this may not be the case. Therefore, the production of coal derived synthesis gas must in turn be subsidized to some extent to make its production economical. These subsidies can take a number of different forms; however, the primary form of subsidy at this juncture is one of by-product credits. If a sufficient level of by-products can be produced in conjunction with the coal derived syngas to compensate for the apparent price differential between the two syngas sources then, the use of coal may be justifiable. Then the question becomes: what level of subsidy is required to make coal derived syngas economical. Before this question can be addressed, the prices for the respective syngases must be derived because they are intermediate products which are not marketed. Consequently, price data does not exist. Thus the primary function of this model is to determine the price of coal and natural gas derived synthesis gas. The model will also be used to evaluate different base cases constructed by the chemical

engineers with respect to their total fixed and variable cost and the effect on output and syngas price. While this model deals primarily with the first stage of the alcohol production process currently, it may easily be adapted to stage two with some minor modifications.

Once the price of syngas from the respective sources has been established, the focus of this investigation may turn to which, if any, potential by-products can provide the appropriate level of subsidies necessary to make coal-use economically feasible.

Alcohol Fuel and By-Products Markets Summary

By-Products

There is virtually an endless array of by-products that may be produced in conjunction with coal derived synthesis gas. Essentially any product that may be obtained from the coking of coal can be a potential by-product of the coal derived syngas production process. However, these product are limited by the technology employed. The potential by-product mix often varies from one type of gasifier to another and also varies with operating conditions. A look at the infamous coal tree shows the potential problems entailed in such a vast market analysis. Therefore, in order to make this task managable the market analysis was performed on broad classifications of value-added coal products which are traded regularly. A time series data base for these products has been developed; however, some gaps still remain due to disclosure problems.

Alcohol Fuels

The potential of methanol as a fuel oxygenate or neat fuel is questionable at best. Its use in this capacity has been marred

by numerous problems ranging from consumer and industry acceptance to its lack of competitiveness. In the early 1980's attempts to use methanol as an octane enhancer resulted in vehicle operation problems attributed in part to phase separation. As a result of these problems, the demand for methanol as a octane enhancer has fallen significantly despite its relative abundance.

Consumption of methanol in gasoline has declined steadily from its high point of 106 million gallons in 1985 to less than 4 million gallons in 1987. By 1988 the demand for methanol as an octane enhancer had become virtually nonexistent.

Historically, this trend has been attributed to methanol's lost cost advantage over other octane enhancers and acceptance problems. Many of the acceptance problems are a result of adverse publicity. Several automobile manufactures stated warranties would not be honored if owners used methanol enhanced gasoline blends in their cars. While these manufactures discouraged the use of gasoline containing methanol as an octane enhancer, they warranted the use of gasoline blends containing up to 10% ethanol. Methanol's acceptance was further eroded by the technical problems such as fuel foaming, aldehydes emissions, vapor locking in hot weather and starting problems in cold weather along with numerous corrosion problems in the engine and fuel system. Reports of these problems prompted the EPA to limit the amount of neat methanol in unleaded gasoline to 0.3% by volume despite the fact that neat methanol concentrations of up to 3 volume % have been used in the Federal Republic of Germany for several years without any reported problems.

The use of ethanol was met with less resistance due in part to the efforts of the corn lobbyist of the Midwest. Initially instituted as a means of conserving crude oil in the late 1970's, a mixture of 10% ethanol and 90% gasoline was used in place of straight gasoline. This procedure soon became

profitable as result of government subsidies and demand for ethanol continued to grow through the 1980's. However, these subsidies only apply to fermentation ethanol and are due to expire at the end of 1992. Without these subsidies which currently amount to about 60 cents-per gallon of ethanol it use a fuel additive would no longer be economically viable. This is because fermentation ethanol, without government subsidies, is the most expensive of all currently used blending agents. Synthetic ethanol is also relatively expensive in comparison to these other blending agents which may account for its lack of use in this market.

The most promising alcohol fuel appears to be tertiary-butyl alcohol (TBA) which is currently approved by an EPA interpretative rule which permits blends approaching 16% by volume for straight TBA. However, ARCO Chemical Company appears to have a monopoly on the production of TBA since 1986. TBA may also be used as a cosolvent with methanol, although its use in this capacity has declined since methanol blending has stopped due to technical problems. The features that make this product so attractive are that it can be used in its original form or it can be further refined to produce high purity isobutylene, which can be reacted with methanol to produce MTBE.

Little can be said about the potential market or value of the proposed mixed alcohol product (Base Case 1), since its exact composition and characteristics are currently unknown. Until some indication of the utility of this product is provided by the fuels engineers, it is virtually impossible to determine its price or demand. Questions of EPA approval may also have to be addressed.

There is little question regarding the potential market for alcohol fuels. The potential local annual market alone is approximately 1700 million gallons used as a 10% blend. The potential problems from the marketing aspect may very well be

regulatory in nature assuming that the alcohol fuel product does not fall into one of the approved categories below. The following table shows the various oxygenated blending agents that are approved by the EPA for use in unleaded gasoline as of September 1990.

TABLE 2 **Oxygenated Blending Agents**

COMPONENT	DESCRIPTION	APPROVED CONCENTRATION
Oxinal ^R	Methanol and gasoline-grade tertiary-butyl alcohol	Limited to 3.5% oxygen by weight in the finished fuel (approximately 9.5% by volume, depending upon the gasoline density).
Arconol ^R	Gasoline-grade TBA (GTBA) (contains small amounts of acetone, butanes, etc.)	Limited to 3.5% oxygen by weight in the finished fuel as a special case of Oxinol above (approximately 16% by volume, depending on gasoline density).

TABLE 2 (CONTINUED)

COMPONENT	DESCRIPTION	APPROVED CONCENTRATION
Methyl-tertiary- Butyl Ether (MTBE)	$C_5H_{12}O$	Limited to 2.7% oxygen by weight in the finished fuel (approximately 15% by volume, depending upon gasoline density).
Du Pont Blend	Mixture of methanol and any one or a combination of ethanol, propanols or butanols (including GTBA) plus Du Pont's corrosion inhibitor DGOI-100	Limited to 3.7% oxygen by weight in the final fuel and limited to a maximum of 5% volume methanol and a minimum of 2.5% co-solvent.
Other Aliphatic Alcohols and Aliphatic Ethers	Aliphatic alcohols: propanols, C_3H_7OH , butanols, C_4H_9OH , etc., except methanol. Aliphatic ethers: TAME, $C_6H_{14}O$, diisopropyl ether, etc.	Limited to 2% oxygen by weight in finished fuel. (Volume proportion varies with the alcohol ether density and the gasoline density.)
Ethanol	C_2H_5OH	Limited to 10% by volume in the finished fuel.

^R Registered trademarks of ARCO Chemical Company

Sources: SRI Chemical Economics Handbook (information on the Du Pont blend)

Petroleum Supply Monthly, EIA Feb.1985 (all other data)

Appendix 4

Fuels Testing

I INSTRUMENTATION

1.1 Engine

A Standard single cylinder CFR spark ignition engine with a variable compression ratio manufactured by Waukesha Motor Company will be used in the experiment. The engine dimensions are given in the Table below

Table 3 CFR spark ignition engine dimensions:

Engine Dimensions	
Compression Ratio Range.....	4:1 to 18:1
Bore, inches.....	3.25
Stroke, inches.....	4.50
Displacement, cubic inches.....	37.33
Valve Port, diameter, inches.....	1.187
Connecting rod bearing:	
diameter, inches.....	2.250
length, inches.....	1.420
Front main bearing:	
diameter, inches.....	3.00
length, inches.....	1.943
Rear main bearing:	
diameter, inches.....	3.00
length, inches.....	3.219
Piston pin, floating, diameter, inches.....	1.25
Connecting rod:	
length, center to center, inches.....	10.00
width, inches.....	1.620
Timing gear face, inches.....	1.00
Exhaust pipe, diameter, inches.....	1.25
Weight of engine, pounds (approximate).....	800

1.2 Ignition system

The ignition system is a condensor-discharged type with coil and distributor. The primary current for the system is supplied by the ignition power pack and 4 micro F condenser. Spark plug used

is Champion D16 with extended electrodes which is set at 0.043 inches gap. A pressure transducer is mounted in the spark plug. A neon-tube ignition spark indicator is placed on the front of the engine to register spark timing.

1.3 Fuel Air System

The CFR engine is equipped with a bowl carburetor, a fuel container, a metering jet, and a fuel level sight glass. The fuel level for a given fuel-air ratio being dependent upon the size of the metering jet. The fuel flow rate is determined as a ratio of fuel consumed, which can be obtained from the level sight glass to the time of consumption which is taken by a timer.

Laminar flow element model 50 MW 20 - 1.5" manufactured by Meriam Instrument will be used to measure the air flow rate. The nominal air flow range of this device is 22 scfm (air at 29.92 "Hg Abs and 70°F) and it has maximum differential pressure of 8 inches H₂O. A valdyne reluctance type differential pressure transducer which connected to 10- 36 V (DC) and RTI/815 board will be used in conjunction with the laminar flow element device. The barometric pressure will be measured using Hg barometer. A Sling psychrometer will be used to measure the relative humidity of the intake air. The intake air temperature will be measured using a thermometer.

1.4 Lubrication System

Lubricating oil formulated by Paramins Technology Div. Exxon Chem. Co. will be used for the experiment. A K-thermocouple will be used to indicate the temperature of the crankcase oil.

1.5 Cylinder Pressure System

To measure cylinder pressure, a dynamic pressure transducer model 111A26 manufactured by PCB Piezotronics will be mounted in the spark plug using model 65. This pressure transducer is low impedance with voltage output (10 mV/psi), and has the range of 0.05 to 500 psi. This transducer will be used in conjunction with PCB-482A charge amplifier.

1.6 Data Processing System

This system consists of:

- PC 486/50 MHz LpMCg RAM
- RTI/815 board, a multifunction analog/digital input/output board. This boards provide data acquisition for 16 single ended or 8 differential channel. This board will be used to record the differential pressure in the laminar flow element, pressure in the cylinder, ignition timing, and temperatures at several places.
- 3 B47-K-04 module, provide linearize and nonlinearized outputs for K thermocouples to be sent to RTI/815 board. This module provides a 0 to 10 Volt output, but has no current output.
- PCB-482A charge amplifier
- K thermocouples which recorded temperature at various location: the H₂O inlet and outlet, exhaust outlet, air inlet, crankcase oil and cylinder. These thermocouple will be connected to 3B47-K-04 module which will send the signal to RTI/815 board.

The layout of this instrumentation is shown in the attached Figure.

Layout of Instrumentation

FIGURE 2

1.7 Gas Sampling

A compact unit to collect bag samples of the exhaust gas has been designed. The single pump unit can be used for both evacuating Tedlar bags and then filling the bags with the exhaust gas during the sampling mode. The integrated sample in the bags will be subsequently analyzed on a analyzer bench (CO , CO_2 , NO_x , O_2 , and total hydrocarbons) that the investigators have built for another project. The unregulated emissions will also be analyzed and the non-methane hydrocarbons will be reported. The schematic of the bag sampling system is presented in the attached figure.

A sampling train for aldehydes and alcohols has also been designed. The unit includes separate sampling streams for aldehydes and alcohols each with its own computer controlled (with a manual control option) mass flow controllers (MFC), pumps, filters and bypass valves. The mass flow controllers rated at 5 slpm are set at a fixed 1.0 lpm when pulling sample across a 2,4 DNPH coated silica gel cartridge. After the sampling is completed the cartridge will be eluted with acidified acetonitrile and analyzed on an HPLC. The alcohol train pulls a sample across a pair of deionized water impingers and the sample is analyzed on a gas chromatograph to measure the oxygenated hydrocarbons in the exhaust. A schematic of the sampling streams is shown in the attached figure.

FIGURE 3

Bag Sampling

Bag Evacuation

Schematic of the Bag Sampling and Evacuation System

FIGURE 4

FORMALDEHYDE AND METHANOL SAMPLING STREAMS

II ENGINE TESTS

Experimental Apparatus and Procedures

The preliminary experiments were done in a standard single cylinder CFR spark ignition engine in the steady state modes of operation. The compression ratio was set at 7.5 and the speed was set at 900 RPM. The preliminary performance tests were conducted to familiarize the investigators with the alcohol blends and their combustion in the I.C. Engine. The fuels tested included 100% gasoline, 10% isobutanol-90% gasoline, 20% isobutanol-80% gasoline, 5% isobutanol-5% methanol-90% gasoline, and 10% isobutanol-10% methanol-80% gasoline. The properties of gasoline, methanol, and isobutanol are listed in Table 1. The gasoline used was Chevron unleaded supreme gasoline. For each run, fuel flow rates were measured volumetrically using a graduated column (incorporated in the CFR engine's fuel system) and a timer, and the air flow rates were determined using a gas flow meter and a timer. For each run, ignition timing was set manually at several values using a standard electronic timing light and the beam loads were recorded at each ignition timing. Minimum advance for best torque (MBT) was determined for each fuel at a fixed compression ratio. Tests were run only at one compression ratio. The final test matrix will include experiments starting with indolene (standard fuel from Phillips 66) and the compression ratio will be changed from 5.5 to the knock limited compression ratio (KLCR) at 900 rpm to determine the minimum advance for best torque (MBT). Then, the alcohol concentration in the indolene will be varied. Performance

parameters such as, brake horse power, brake specific fuel consumption and brake thermal efficiency will be calculated. Additionally, flame speeds and burning velocity will also be determined. During each run fuel flow rate, air flow rate, exhaust temperature, torque, exhaust emissions, air inlet temperature, rpm, etc. will be calculated. No emissions analysis was done in this quarter. However, the instrumentation for collecting the bag samples was tested.

Table 4. Gasoline, Methanol, and Isobutanol Properties (Bata, 1989)

Property	Gasoline unleaded	Butanol C_4H_9OH ISO	Methanol CH_3OH
Approximate Specific gravity at 60°F	0.72-0.75	0.81	0.79
Boiling point			
°F	85-437	226.6	149
°C	30-225	108.1	65
Net Lower Heating Value (mass)			
Btu/lbm	18,700	14,280	8,600
MJ/kg	43.5	33.0	20.1
Net Lower Heating Value (volume)			
Btu/gal	117,000	95,880	57,000
MJ/l	32	26.0	15.9
Heat of Vaporization			
Btu/gal	170	253.7	500
KJ/kg	400	579	1,100
Vapor Pressure at 100°F			
psi	9-13	0.62	4.6
kPa	62-90	2.25	32
Octane Number			
Research	91-100	113	112
Motor	82-92	94	91
Stoichiometric A/F ratio	14.6	11.1	6.4
Vapor Flammability limits, volume	0.6-8	1.8-8.4	5.5-26
Viscosity at 104°F (40°C)			
Centipoise	0.5	1.45	0.46
Centistoke	0.6	1.92	0.58
Appearance	Colorless	Colorless	Colorless
Vapor Toxicity	M.Irritant	Irritant	Irritant

Figure 5. A/F vs. Alcohol Concentration

RESULTS AND DISCUSSION

Air Fuel Ratio

Figure 5 and Table 5 show the air fuel ratio as a function of alcohol concentration. The results from this experiment were not as expected. Figure 1 shows that the air/fuel ratio increases as the alcohol concentration in the blend increases. It is expected that as the alcohol concentration increases, air/fuel ratio decreases. It may be noted that this behavior is apparant in both the blends. However, as expected, the isobutanol-gasoline mixture air/fuel ratios are higher than that of isobutanol-methanol-gasoline mixture.

Table 5. Air Fuel Ratio for Each Fuel (Mass Bases)

Fuel	Air/Fuel Ratio
Gasoline	9.24
10%Isobutanol-90%Gasoline	10.34
20%Isobutanol-80%Gasoline	10.51
5%Isobutanol-5%Methanol-90%Gasoline	10.26
10%Isobutanol-10%Methanol-80%Gasoline	9.53

Figure 6 MBT vs. Alcohol Concentration

Effect of Alcohol on MBT Spark Advance

Figure 6 and Table 6 shows the effect of varying methanol and isobutanol fraction on the MBT spark advance at compression ratio of 7.5:1. At a fixed compression ratio, as the alcohol concentration increases, the MBT spark timing shifts toward top dead center. The MBT spark advance of gasoline-isobutanol blends is lower than that of gasoline-isobutanol-methanol blends. The gasoline-alcohol blends are expected to yield a higher burning velocity compared to gasoline and isobutanol-methanol-gasoline blends. When additional tests are conducted at different compression ratios, it is expected that the MBT spark timing will shift toward TDC.

Table 6 . MBT for Each Fuel

Fuel	MBT
Gasoline	26
10%Isobutanol-90%Gasoline	24
20%Isobutanol-80%Gasoline	22
5%Isobutanol-5%Methanol-90%Gasoline	25
10%Isobutanol-10%Methanol-80%Gasoline	24

REFERENCES

1. Bata, Reda M., Alvon C. Elrod and Thomas P. Lewandowski.
"Butanol as a Blending Agent with Gasoline for I.C. Engine."
SAE Paper No. 890434.
2. Patel, K. S., S. Kumar, and O. Y. Kwon. "The Performance
Characteristics of Indolene-MPHA Blends in a Spark Ignition
Engine." SAE Paper No. 872068.

END

**DATE
FILMED**

12/23/93