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

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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 gasifer 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 ("$MoNN_3Py$").

<u>Approach 1</u>

Based on a literature review, the following organometallic compounds have been selected for evaluation: $Cp^*_2Mo_2Fe_2(CO)_8$, $Cp_2Mo_2Co_2S_3(CO)_4$, $Cp_2Mo_2Ni_2S_4(CO)_2$, $Cp_2Mo_2Co_2S_4(CO)_2$, $Cp_2Mo_2Fe_2)S_4(CO)_6$, $(NEt_4)_2\{M(SPh)_4[Mo(CO)_4]_2$ (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 $(NH_4)_2Mo_3S_{13}$ 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% $NH_3(aq)$) to 20 ml of an ammonium molybdate solution (prepared by dissolving 4.0 g of $(NH_4)_6Mo_7O_{24}\cdot 4H_2O$ in 20 ml of water) and heating for 5 days at 95 °C. $(NH_4)_2Mo_3S_{13}$ 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 ($K_2Mo_3S_{13}$) has also been made by a similar procedure where a potassium polysulfide solution was used instead of the ammonia solution. $(NH_4)_2MoS_4$ has been obtained for use in the preparation of supported Chevrel phase compounds.

Approach 3

The starting materials, $Mo(CO)_6$ and $Co_2(CO)_8$ have been obtained and sublimed for use. $Fe(CO)_5$, $NbCl_5$, $TaCl_5$ $ZrCl_4$, $HfCl_4$ 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.

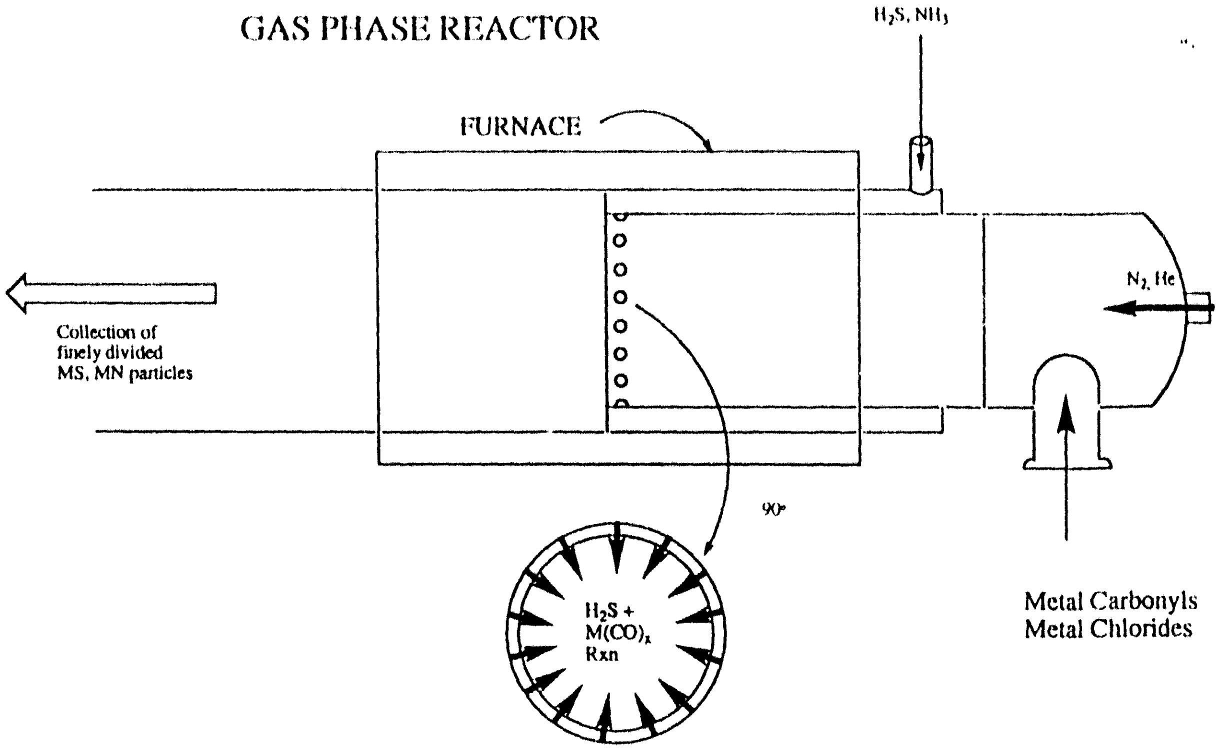


Figure 1.1 Diagram of a quartz reactor comprised of two concentric quartz tubes (56 mm and 48 mm) for reaction of volatile metal compounds with reactive gases, specifically H_2S. The volatile metal compounds (e.g., $Mo(CO)_6$ or $Co_2(CO)_8$) will be sublimed into the He carrier gas. H_2S will be introduced 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:

$$Mo_2(CH_3CO_2)_4 + 8\ (CH_3)_3SiN_3 \longrightarrow Mo_2(N_3)_4Py_4 + 4(CH_3)_3SiO_2CCH_3$$
$$Mo_2(N_3)_4Py_4 \longrightarrow \text{"MoNN}_3\text{Py"}$$

Thermal decomposition of "$MoNN_3Py$" 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. N_2 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 $MoNN_3Py$ 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 N_2 Adsorption/Desorption Surface Area Studies of $MoNN_3Py$ 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 thoria 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 lements 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)**

$$\frac{dN_j}{dt} = W\sum_{i=1}^{nr} \upsilon_{ij} r_i \text{ , } N_j(o) = N_{jo} \text{ ; } j = 1, 2, \ldots, nc.$$

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

$$\frac{dN_j}{dt} = F_{jo} - F_j + W\sum_{i=1}^{nr} \upsilon_{ij} r_i \text{ , } N_j(o) = N_{jo} \text{ ; } j = 1, 2, \ldots, nc.$$

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

$$\frac{dF_j}{dW} = \sum_{i=1}^{nr} \upsilon_{ij} r_i \text{ ; } F_j(o) = F_{jo} \text{ ; } j = 1, 2, \ldots, nc.$$

where

N_j : moles of component j at any time

N_{jo} : moles of component j present initially

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

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

υ_{ij} : stoichiometric coefficient for component j in the ith 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 :**

$CO + 2H_2 \rightleftharpoons CH_3OH$ (1)

$CH_3OH + (N_C - 1)\,CO + 2\,(N_C - 1)\,H_2 \longrightarrow HA + (N_C - 1)H_2O$ (2)

$CO + H_20 \rightleftharpoons CO_2 + H_2$ (3)

$CO + 3H_2 \longrightarrow CH_4 + H_2O$ (4)

$HA \longrightarrow OL + H_2O$ (5)

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 :**

$$r_1 = k_1 \left[p_{CO}\, p_{H_2}^{2} - \frac{p_{CH_3OH}}{K_1} \right] ; \qquad r_4 = k_4\, p_{H_2}$$

$$r_2 = \frac{k_2\, p_{CH_3OH}}{\left[1 + K_W\, p_{H_2O} \right]} ; \qquad r_5 = k_5 \left[p_{HA} \right]^{\frac{1}{2}}$$

$$r_3 = k_3 \left[p_{CO}\, p_{H_2O} - \frac{p_{CO_2}\, p_{H_2}}{K_3} \right]$$

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)

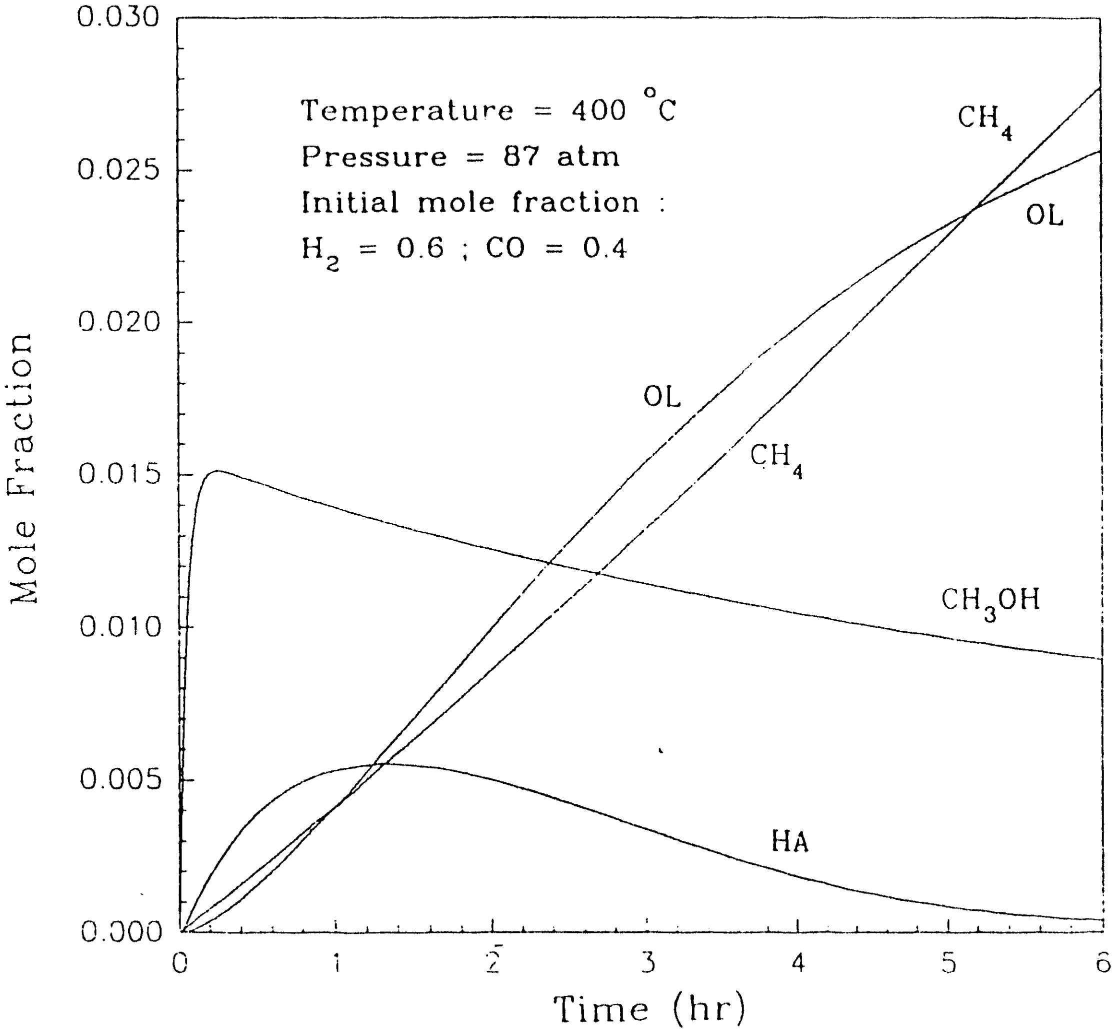


Figure 1.3

PLUG-FLOW TUBULAR REACTOR (PFTR)

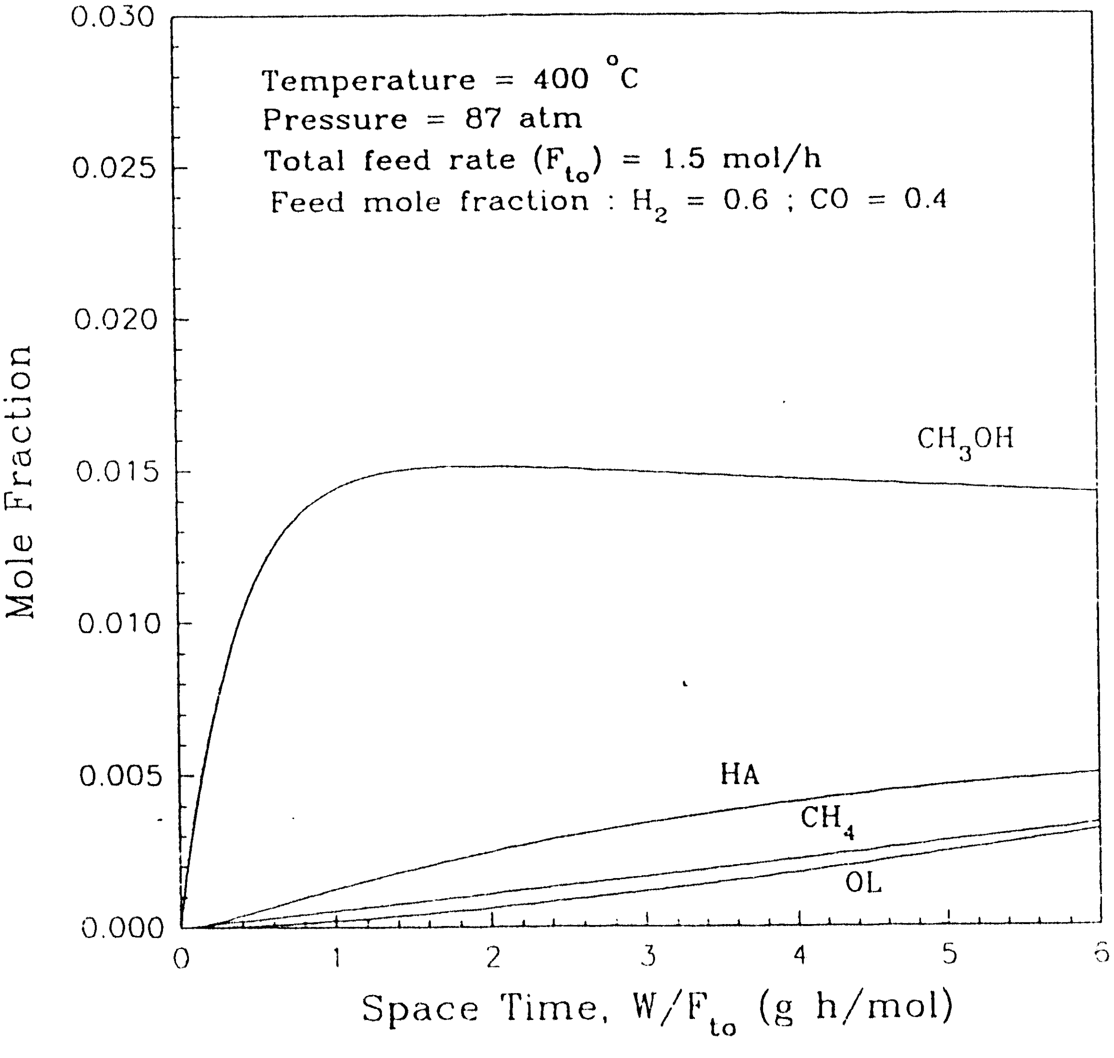


Figure 1.4

CONTINUOUS STIRRED-TANK REACTOR (CSTR)

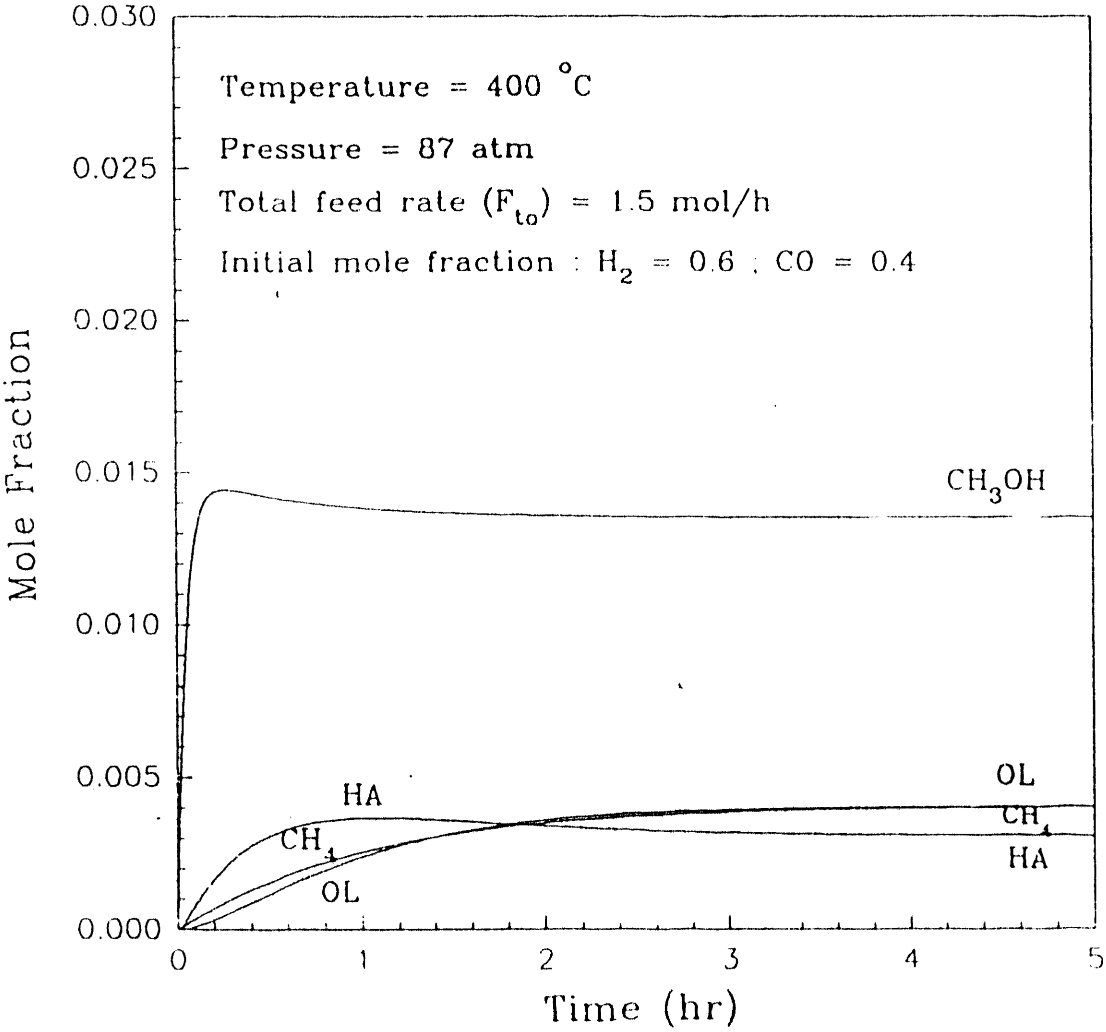


Figure 1.5

CONTINUOUS STIRRED-TANK REACTOR (CSTR)

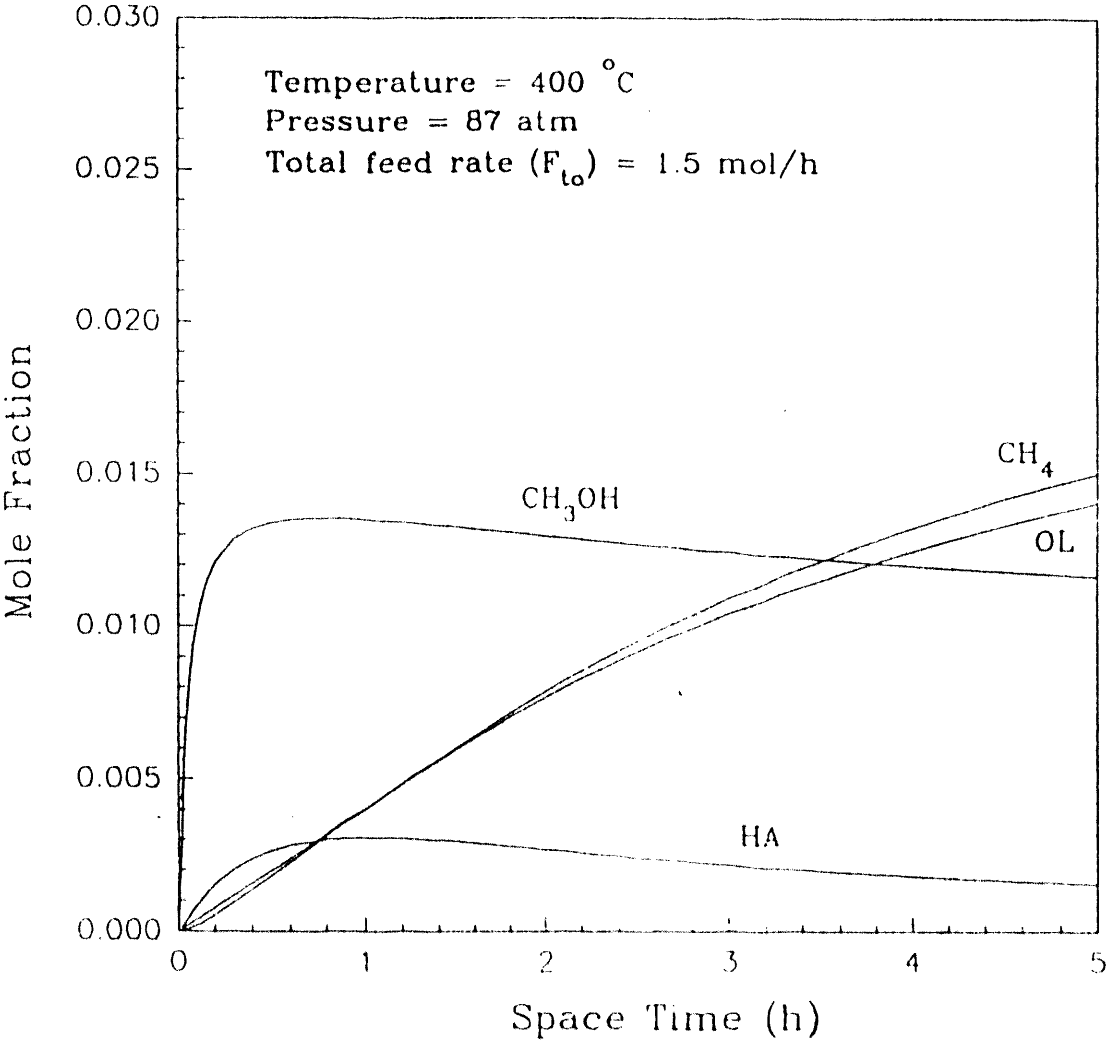


Figure 1.6

PERFECTLY-MIXED BATCH REACTOR (PMBR)

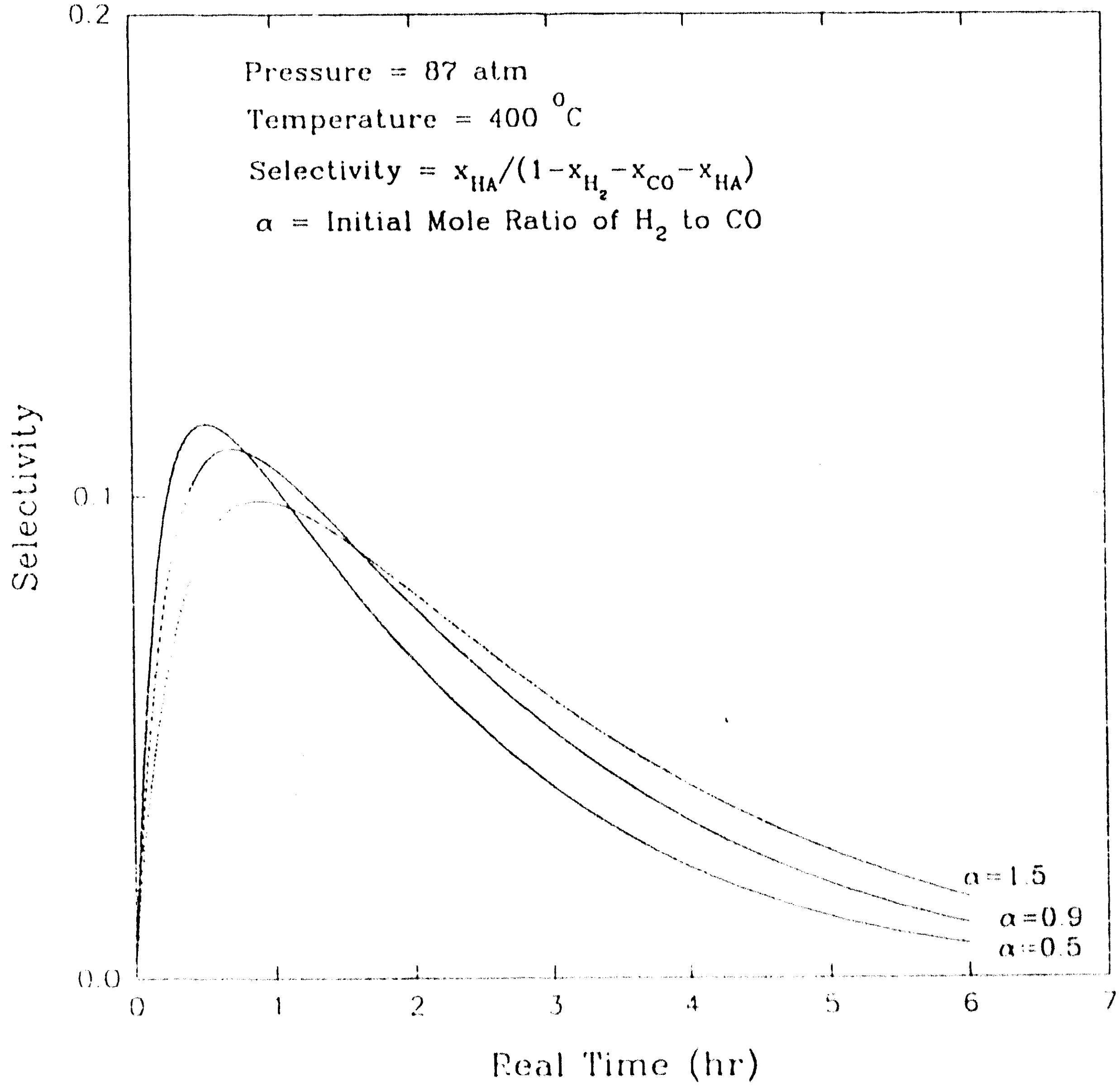


Figure 1.7

PLUG-FLOW TUBULAR REACTOR (PFTR)

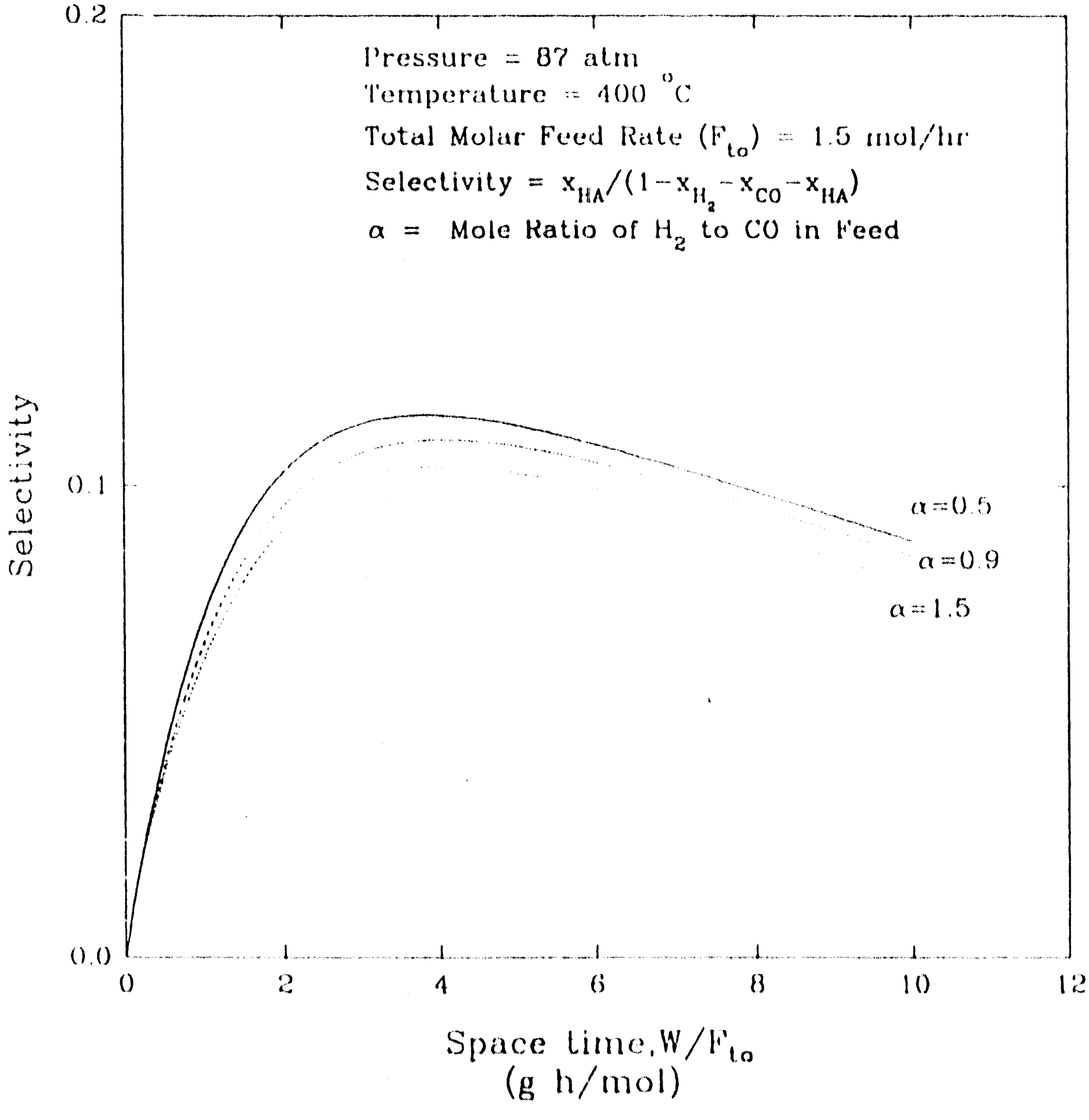


Figure 1.8

CONTINOUS STIRRED-TANK REACTOR (CSTR)

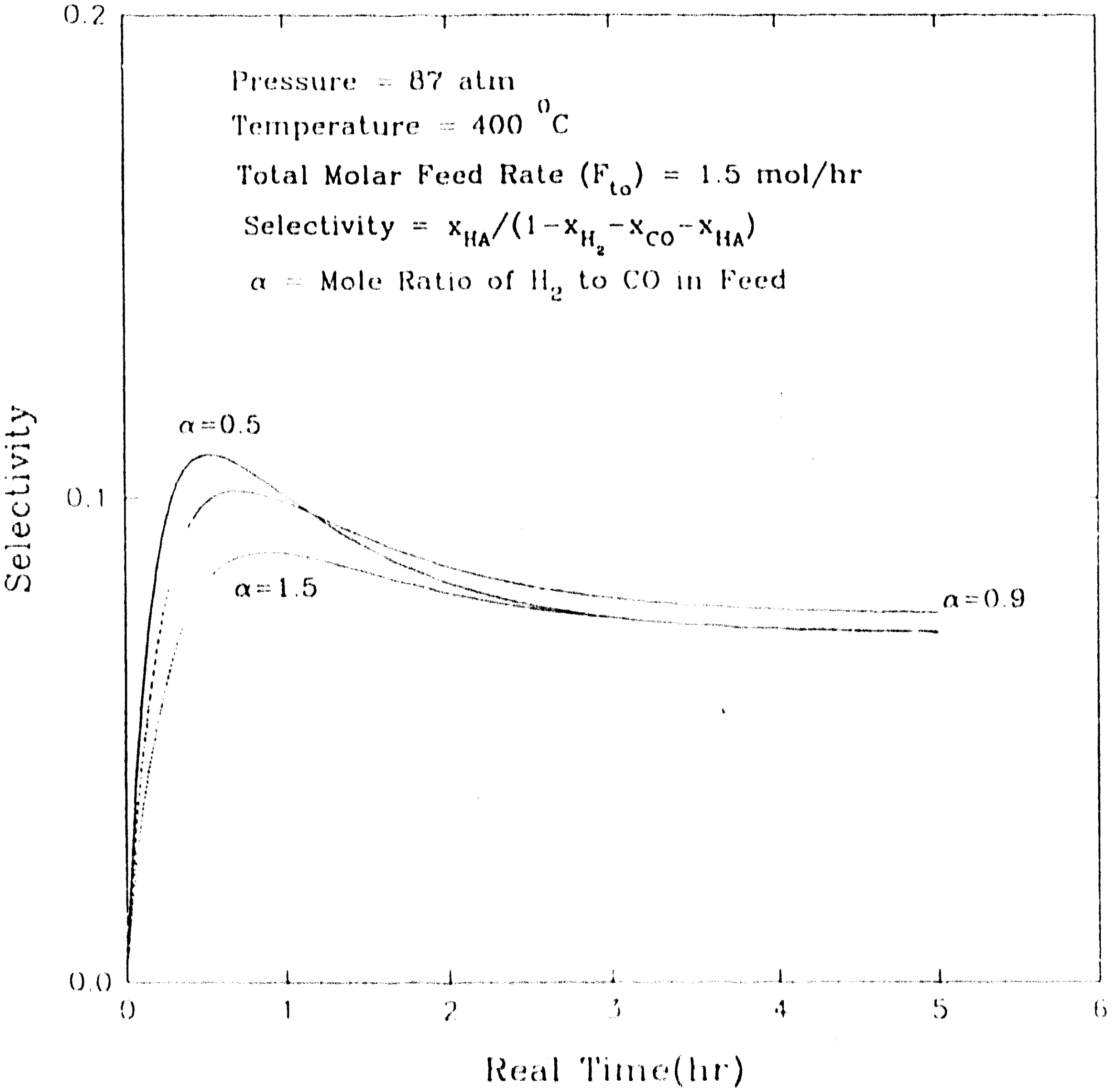
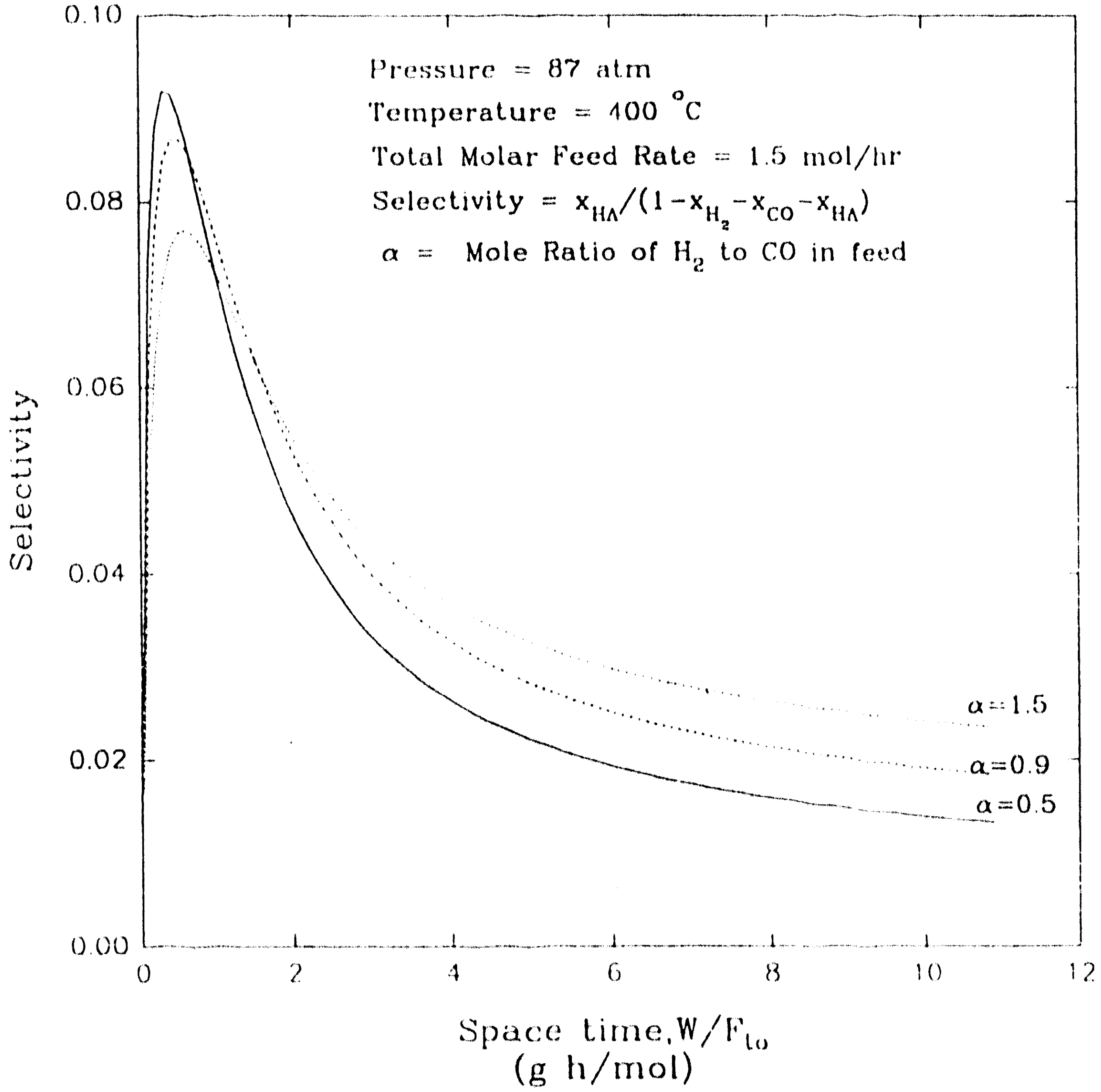


Figure 1.9

CONTINOUS 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 Cu0.63 Ce0.18 Zr0.09 K0.1 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

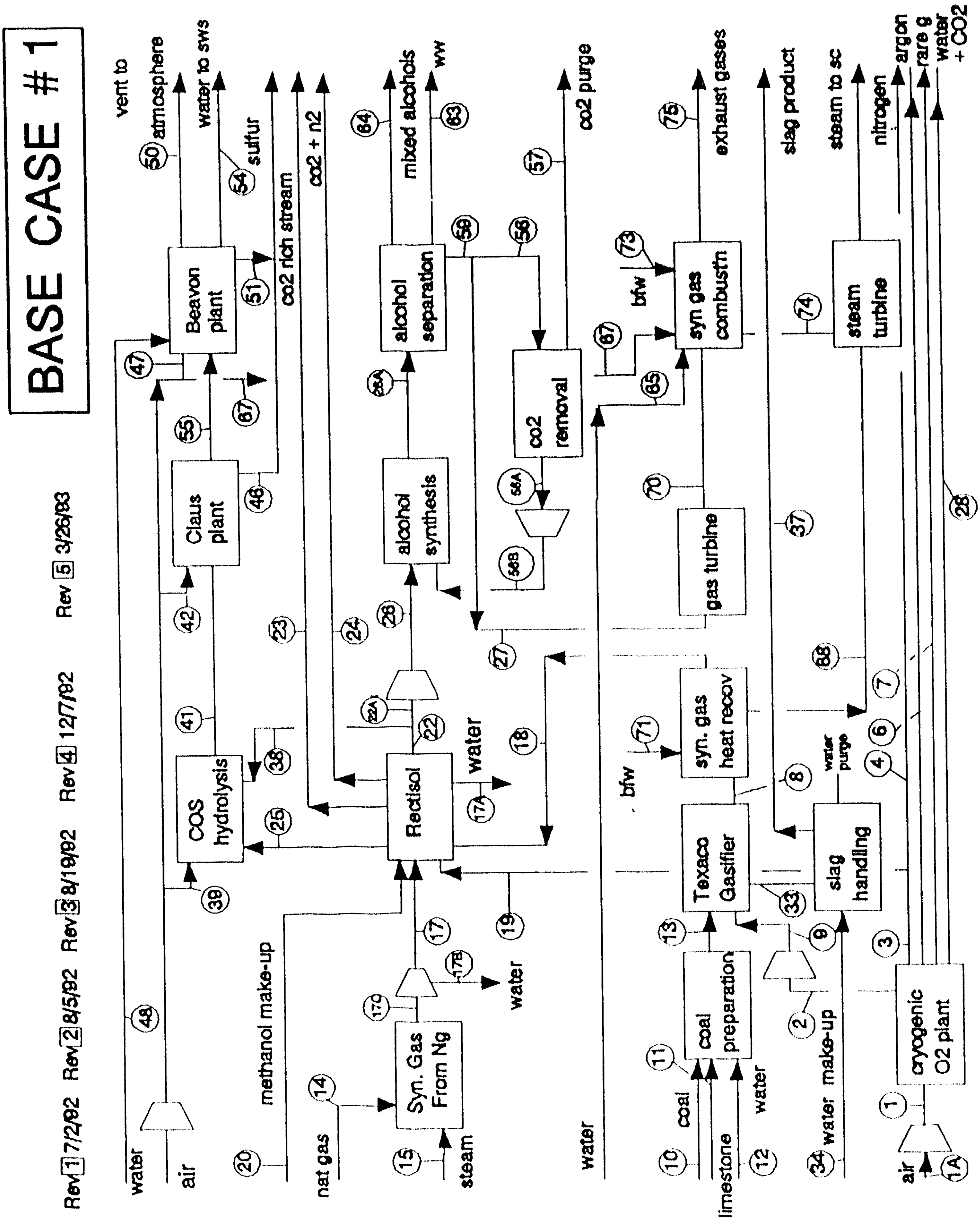
Synthesis Gas via Methane	16.8
Coal Preparation	47.7
Texaco Gasifier	163.7
Slag Handling	3.0
Steam/Power Generation	89.3
Synthesis Gas Heat Recovery	7.8
Cryogenic Oxygen Production	76.7
Rectisol(Acid Gas Separation)	38.2
COS Hydrolysis	
Claus (Sulfur Recovery)	11.1
Beavon	4.2
MoS_2 Alcohol Synthesis 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.



FLO. CHART FOR BASE CASE 1 - 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	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	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	4.6	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	260634.1	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	251.2	251.2	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	89.2	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
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	0.3	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
Kmol/hr	109.8	251.2	251.2	109.8	99.3	121.2	163.5	152.2	302.2	64.8
Kg/hr	11190.4	4521.6	4521.6	11190.4	1426.0	3520.4	6198.8	4422.4	9181.7	2073.6
Temp (C)	1300.0	25.0	156.0	156.0	25.0	25.0	25.0	25.0	370.0	370.0
Press.(KPA)	8135.8	3447.4	3000.0	103.4	8106.0	15.0	15.0	103.4	103.4	103.4

TABLE 1.1 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	8329.5	8329.5	8329.5	0.0	8329.5
H2O	0.0	20.0	0.0	0.0	72.0	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	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	8.3	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
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	0.0	0.0	0.0	464.0
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	283974.8
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

	063	064	065	067	068	070	071	073	074	075
Ar	0.0	0.0	0.0	62.0	0.0	0.0	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	0.0	0.0
CH3OH	0.0	622.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C2H5OH	0.0	649.4	0.0	0.0	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	0.0	0.0
C4H9OH	0.0	36.2	0.0	0.0	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	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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	498.6
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	138.7	0.0	422.5	0.0	9626.4	0.0	9626.4	6200.0	6200.0	1402.4
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	4827.6	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	1292.0	0.0	0.0	0.0	0.0	0.0	303.4
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	17.9	0.0	0.0	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	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	464.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	17.3	0.0	0.0	0.0	0.0
kmol/hr	168.4	1466.8	422.5	6181.6	9626.4	0.0	9626.4	6200.0	6200.0	7094.0
kg/hr	4859.6	62413.2	7605.0	178996.8	173275.2	7943.0	173275.2	111600.0	111600.0	194543.2
Temp.(C)	25.0	25.0	25.0	25.0	482.0	25.0	20.0	20.0	482.2	25.0
Press.(KPA)	11666.0	11666.0	103.4	103.4	10000.0	101.3	10000.0	10000.0	10400.0	101.3

TABLE 3.1 - CONTINUED

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_2 Alcohol Synthesis Loop	40.0
CO_2 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.

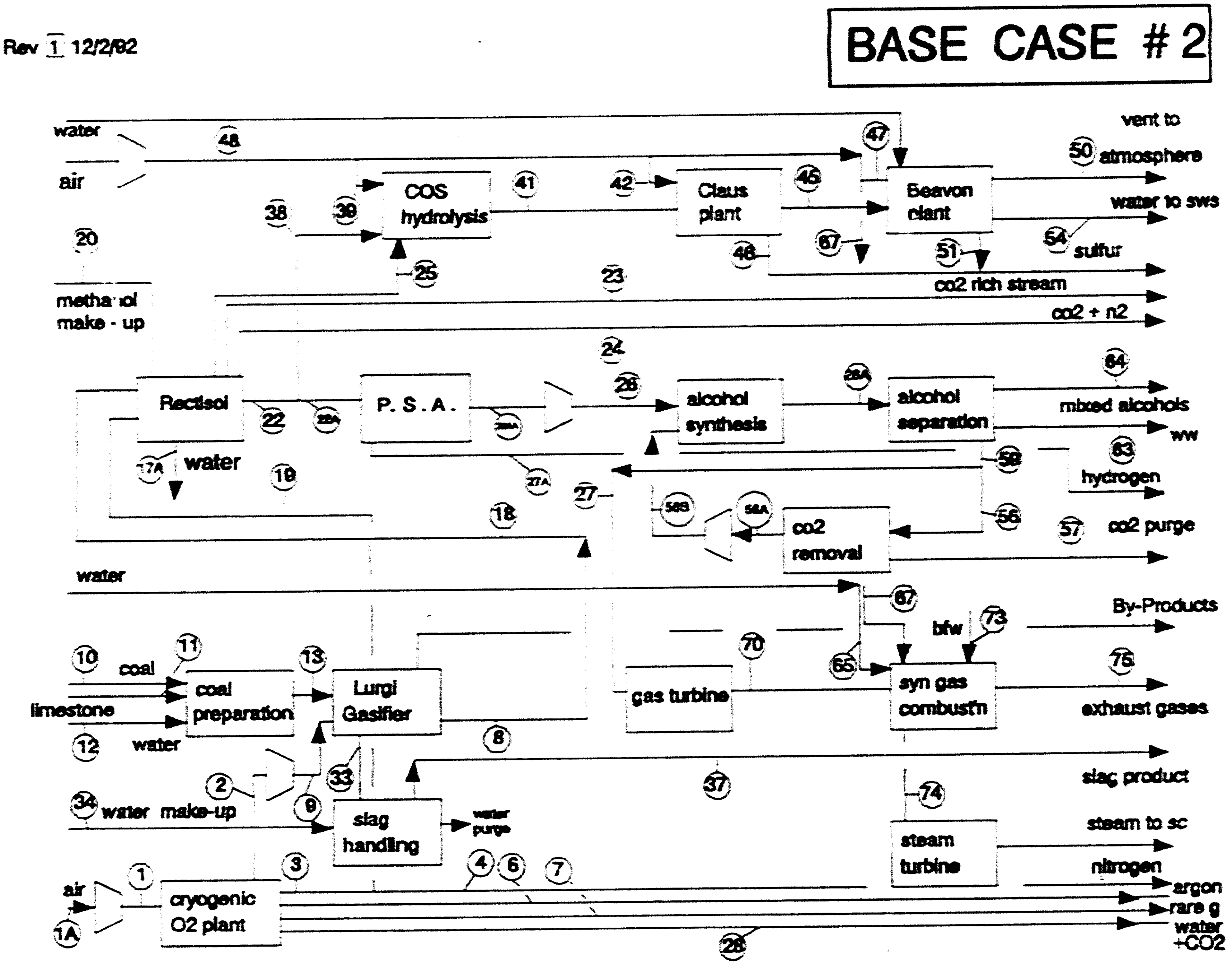


FIGURE 2.2 FLOW CHART FOR BASE CASE 2

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

	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	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	6395.1	0.0	0.0	0.0	0.0	0.0	3837.1
COS	0.0	0.0	0.0	8.4	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	11123.0	0.0	0.0	11123.0	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	18.0	18178.0	17996.5	12188.9	3837.1
kg/hr	483120.0	767077.6	353124.0	836470.5	280532.0	576.0	191192.4	189282.0	312981.2	168832.4
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	517.1	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 ($85/m')	100.5	
Other Expenses	42.0	
TOTAL ESTIMATED CREDITS (EXCLUDING ALCOHOLS)(MM$/YR)		29.5
Power ($0.05/kW-hr)	29.5	

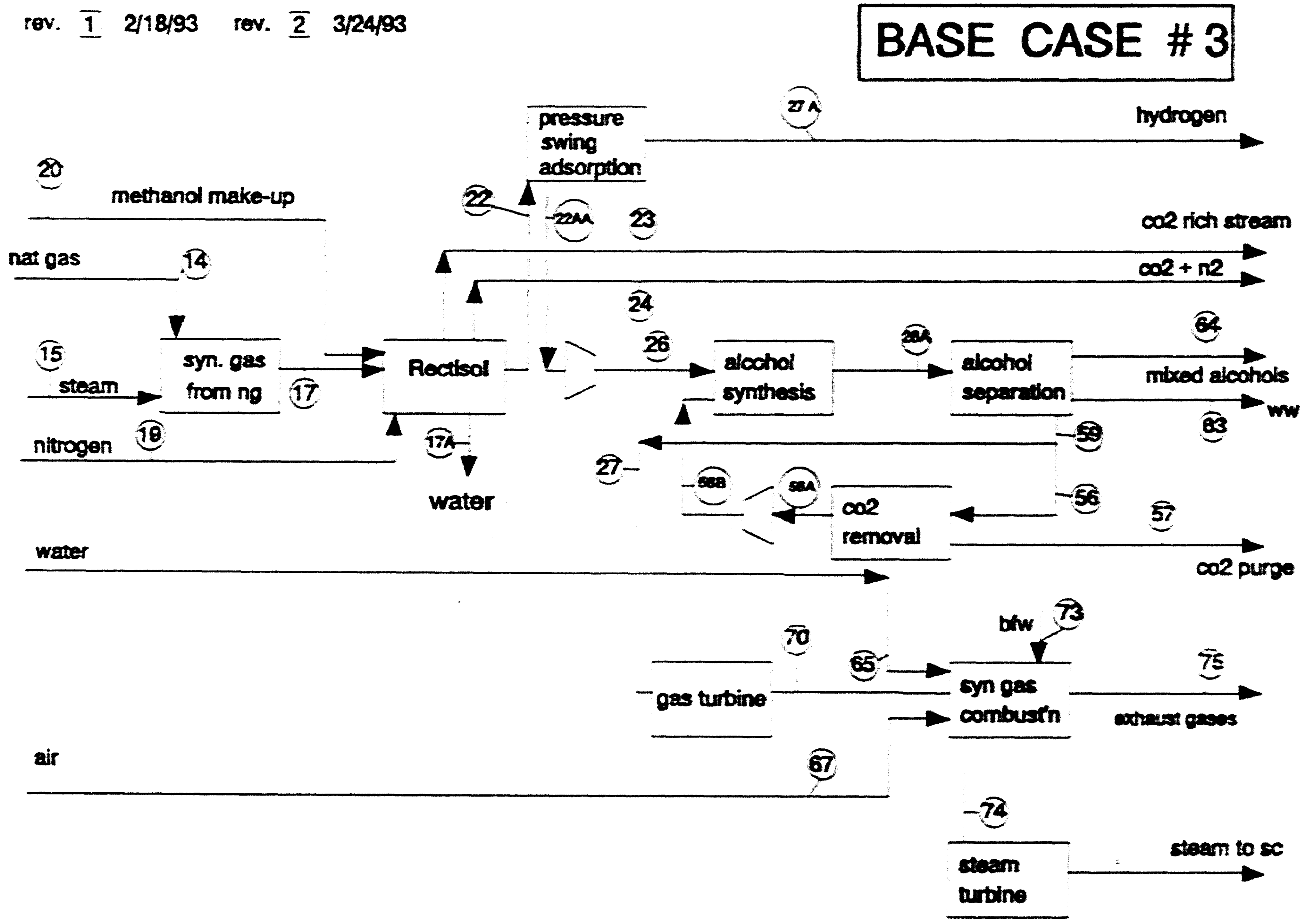


FIGURE 2.3 FLOW CHART FOR BASE CASE 3

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
C3H7OH	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
C5H11OH	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	402.2
COS	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	16558.0	0.0	0.0	0.0	16558.0	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
NH3	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
Al2O3	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
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	202.0	8106.0	207.0	103.4	8106.0	8106.0	8106.0

TABLE 2.3 FLOW TABLE FOR BASE CASE 3

	024	026	026A	027	27A	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	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	1479.9	0.0	0.0	1479.9	1479.9
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	5207.3	8366.2	0.0	11350.0	8362.8	8362.8	8362.8	0.0	8362.8
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
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	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	9832.9	18873.0	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	283598.2
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	14185.0	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
COS	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	1248.8
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
C3H6O2	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	62405.6	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)	12666.0	12666.0	103.4	103.4	101.3	10446.0	10446.0	101.3

TABLE 2.3 (CONTINUED)