

2.2.5 Base Case 4

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

2.2.5.1 Stand Alone Compressors and Power Summary for Base Case 4

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

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

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

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

2.2.5.3 Overall Economic Evaluation for Base Case 4

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

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

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

BASE CASE # 4

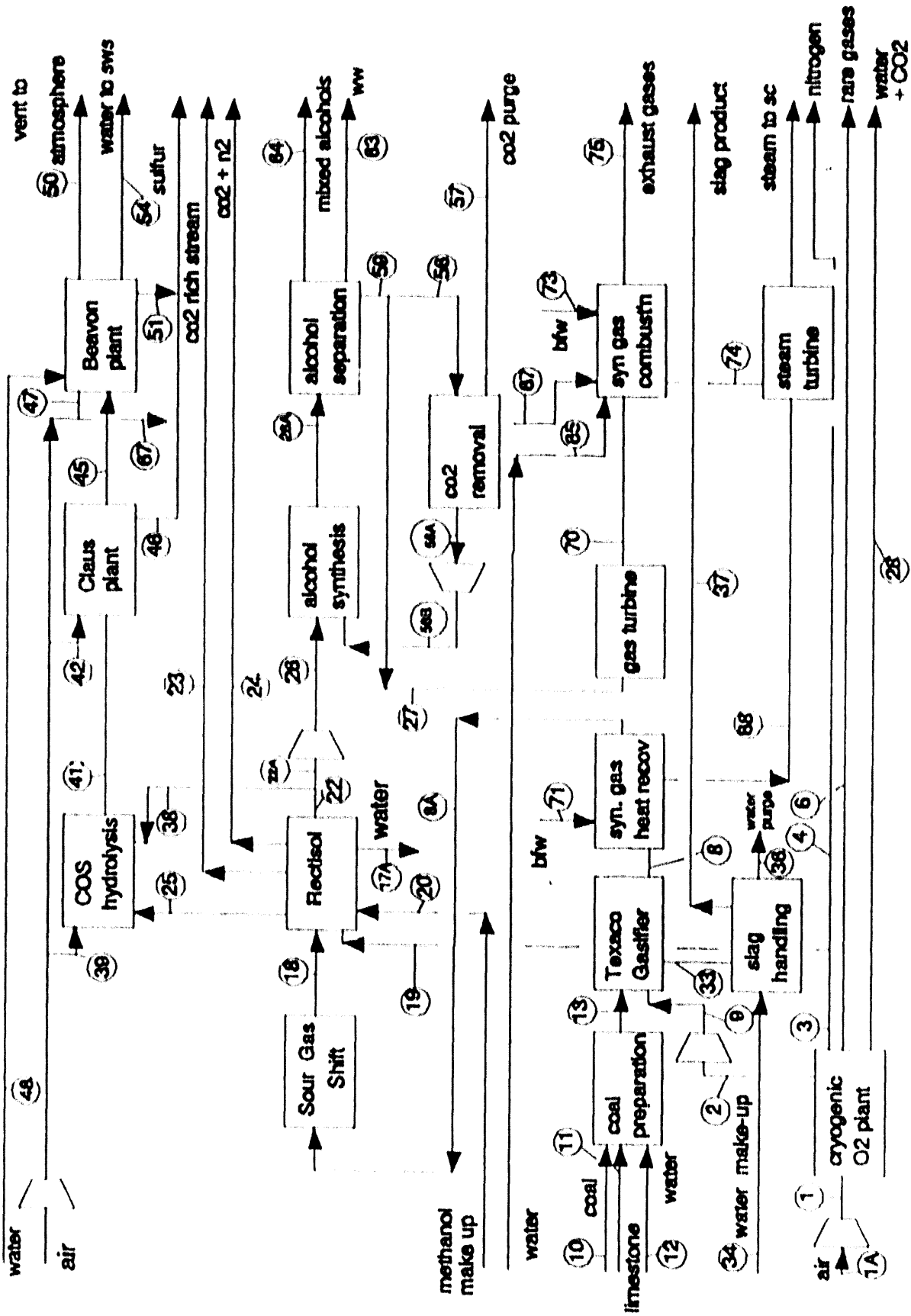


FIGURE 2.4 FLOW CHART FOR BASE CASE 4

Base Case #	CC1	CC1A	CC2	CC3	CC4	CC6	CC8	8a	CC9	CC0
AZ	154.5	154.5	0.0	0.0	0.0	154.5	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-322.7
CR30R	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CR50R	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CR70R	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CR90R	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CR100R	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CC	0.0	0.0	0.0	0.0	0.0	0.0	575.3	575.3	0.0	0.0
CC1	5.8	5.8	0.0	0.0	0.0	0.0	2055.2	2055.2	0.0	0.0
CC5	0.0	0.0	0.0	0.0	0.0	0.0	4.9	4.9	0.0	0.0
CC60	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CC	0.0	0.0	0.0	0.0	0.0	0.0	4214.1	4214.1	0.0	3156.6
CC1	425.4	425.4	0.0	0.0	0.0	0.0	5420.0	5420.0	0.0	50.0
CC5	0.0	0.0	0.0	0.0	0.0	0.0	100.1	100.1	0.0	0.0
CC60	1370.0	1370.0	0.0	1370.0	716.4	0.0	63.5	63.5	0.0	68.2
CC	0.0	0.0	0.0	0.0	0.0	0.0	11.5	11.5	0.0	0.0
CC1	3704.9	3704.9	3704.9	0.0	0.0	0.0	0.0	0.0	3704.9	616.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	105.0
AL203	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	146.6
CR502	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CR802	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CR4	0.0	0.0	0.0	0.0	0.0	0.0	37.2	37.2	0.0	0.0
CR6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
AL202/AL	1800.6	1800.6	3704.9	1370.0	716.4	164.5	27631.9	27631.9	3704.9	12046.1
AL2	11859.2	11859.2	118556.8	39594.0	200519.2	6580.0	362861.5	362861.5	118556.8	141848.4
Temp. (C)	262.0	25.0	25.0	25.0	25.0	25.0	1300.0	25.0	40.0	25.0
Press. (KPA)	510.0	102.0	510.0	510.0	510.0	204.0	8030.0	8030.0	8030.0	102.0

TABLE C-1 FROM TABLE FOR BASE CASE #

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

TABLE 2.4 (CONTINUED)

	024	025	026	026A	027	028	033	034	036	037
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	18.0	0.0	622.6	0.0	0.0	0.0	0.0	0.0	0.0
C2H6O	0.0	0.0	0.0	649.4	0.0	0.0	0.0	0.0	0.0	0.0
C3H8O	0.0	0.0	0.0	143.7	0.0	0.0	0.0	0.0	0.0	0.0
C4H10O	0.0	0.0	0.0	36.2	0.0	0.0	0.0	0.0	0.0	0.0
C5H12O	0.0	0.0	0.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	0.0	4625.9	6937.9	0.0	0.0	0.0	0.0	0.0	0.0
CO2	1087.8	155.4	0.0	1480.1	0.0	5.8	0.0	0.0	0.0	0.0
COS	0.0	4.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	6.4	0.0	0.0	6.4
H2	0.0	0.0	5204.4	7806.4	0.0	0.0	0.0	0.0	0.0	0.0
H2O	0.0	0.0	0.0	138.8	0.0	425.4	0.0	349.7	349.7	0.0
H2S	0.0	100.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	6682.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NH3	0.0	11.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	146.6	0.0	0.0	146.6
C3F6O2	0.0	0.0	0.0	17.9	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	11.8	0.0	0.0	0.0	0.0	0.0	0.0
CH4	0.0	0.0	36.7	473.8	473.8	0.0	0.0	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	17.3	17.3	0.0	0.0	0.0	0.0	0.0
kmol/hr	7769.9	289.9	9867.0	18350.9	491.1	431.2	153.0	349.7	349.7	153.0
kg/hr	234962.0	11012.5	140521.2	350376.0	8099.8	7912.4	15593.2	6294.6	6294.6	15593.2
Temp.(C)	25.0	25.0	310.0	310.0	50.0	25.0	1300.0	25.0	156.0	156.0
Press.(KPA)	102.0	102.0	14000.0	14000.0	14000.0	204.0	8030.0	3400.0	3400.0	102.0

TABLE 2.4 (CONTINUED)

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

TABLE 2.4 (CONTINUED)

	054	056	056A	056B	057	059	063	064	065	067
Ar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	52.0
C	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH3OH	0.0	0.0	0.0	0.0	0.0	0.0	0.0	622.6	0.0	0.0
C2H6O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	649.4	0.0	0.0
C3H8O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	143.7	0.0	0.0
C4H10O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	36.2	0.0	0.0
C5H12O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0	0.0	0.0
CO	0.0	6937.9	6937.9	6937.9	0.0	6937.9	0.0	0.0	0.0	0.0
CO2	0.0	1480.1	0.0	0.0	1480.1	1480.1	0.0	0.0	0.0	0.0
COS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaCO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	7806.3	7806.3	7806.3	0.0	7806.3	0.0	0.0	0.0	0.0
H2O	100.1	0.0	0.0	0.0	0.0	0.0	138.8	0.0	422.5	0.0
H2S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
N2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4827.6
NH3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	242.0
S	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C3H6O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8O2	0.0	0.0	0.0	0.0	0.0	0.0	17.9	0.0	0.0	0.0
CH4	0.0	0.0	0.0	0.0	0.0	0.0	11.8	0.0	0.0	0.0
C2H6	0.0	0.0	0.0	0.0	0.0	473.8	0.0	0.0	0.0	0.0
kmol/hr	100.1	16224.3	14744.2	14744.2	1480.1	16698.1	168.5	1466.9	422.5	6231.6
kg/hr	1801.8	274998.2	209873.8	209873.8	65124.4	282579.0	4861.4	62416.4	7605.0	177396.6
Temp. (C)	370.0	310.0	310.0	310.0	25.0	310.0	25.0	25.0	25.0	25.0
Press. (KPA)	102.0	12500.0	12500.0	14000.0	102.0	12500.0	102.0	102.0	102.0	102.0

TABLE 2.4 (CONTINUED)

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

TABLE 2.4 (CONTINUED)

2.2.6 Discussion of Base Cases

2.2.6.1 Economic Comparison of the Base Cases

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

Base Case 1 - Texaco Gasification and Steam Reformation

Base Case 2 - Lurgi Gasification

Base Case 3 - Steam Reformation Only

Base Case 4 - Texaco Gasification Only

(all costs in MM\$)	Case 1	Case 2	Case 3	Case 4
Cryogenic Oxygen Plant	76.7	139.9	-	82.6
Coal Preparation	47.7	91.9	-	51.8
Gasification	163.7	269.7	-	188.1
Slag Handling	3.0	5.9	-	3.3
Heat Recovery	7.8	-	-	8.4
Power Generation	89.3	166.7	51.5	83.1
Compressors	40.9	40.0	13.7	31.0

Rectisol	38.2	121.9	18.7	41.1
Claus	11.1	21.5	-	12.0
Beavon	4.2	8.1	-	4.5

Steam Reformer	16.8	-	62.5	-
Pressure Swing Adsorption	-	10.0	10.0	-
Sour Gas Shift Converter	-	-	-	6.7

Alcohol Synthesis	40.0	40.0	40.0	40.0
CO ₂ Removal	15.6	15.6	15.6	15.6
Total	555.0	931.2	212.0	568.2

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

Gasification Blocks

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

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

Case 1 and Case 4 economics are very similar, and they will be referred to as Case 1,4 unless a comparison between them is required. The cost of the Cryogenic Oxygen Plant is almost double in Case 2 over Case 1,4 because of the increased coal feed required. The Lurgi Gasification System produces value-added by-products, but as a consequence it also produces large amounts of CO₂. Thus it is necessary to feed about three times as much coal to produce the same amount of syngas and, therefore, the same amount of mixed alcohols. For the same reason, the cost of the Coal Preparation, Gasification, and Slag Handling blocks are all similarly much higher. The above blocks, including the Cryogenic Oxygen Plant, are not required for Case 3. The heat recovery block is designed to produce 10000 kPa steam, which is only done in Case 1,4 because in Case 2 the gasification temperature is not high enough and in Case 3 no coal is gasified. The cost of the Power Generation block is a function of the gross power produced in this section, which is a function of the amount of methane produced in the process and the amount of 10000 kPa steam produced in the Heat Recovery block. A fixed amount of methane is generated in the Alcohol Synthesis Reactor, addition 10000 kPa steam is produced in the Case 1,4 Heat Recovery System, slightly increasing the cost, and in Case 2 a large amount of methane is produced in the Gasification Block which greatly increases the capital cost. The additional compressors in each plant are all roughly the same cost with the exception of Case 3 because no air compressor or oxygen compressor is required because no Cryogenic Oxygen Plant is required.

Acid Gas Cleanup and Sulfur Removal

The cost for the Rectisol block is largely a function of the CO₂ that must be removed. For this reason the cost of this block in Case 2 is far greater than the other blocks. Case 1,4 is next, while Case 3 is very low because the Steam Reformation system produces a much lower amount of CO₂ than either the Lurgi or the Texaco system. The cost of the Claus and Beavon Sulfur removal blocks is directly attributable to the amount of coal fed to the plant, so again, the Case 2 blocks are more expensive than the Case 1,4 blocks. Case 3 has no coal feed and thus no sulfur to remove.

Syngas H₂:CO Ratio Adjustment

Case 1 requires a steam reformer to make a high H₂:CO ratio gas to mix with the low ratio gas from the gasification block. Case 3 uses a reformer to generate all of its syngas and then removes the excess hydrogen with a Pressure Swing Adsorption block, as does Case 2 (The Lurgi gasifier produces a high H₂:CO

PAYBACK PERIOD FOR WUTASK2 BASE CASES

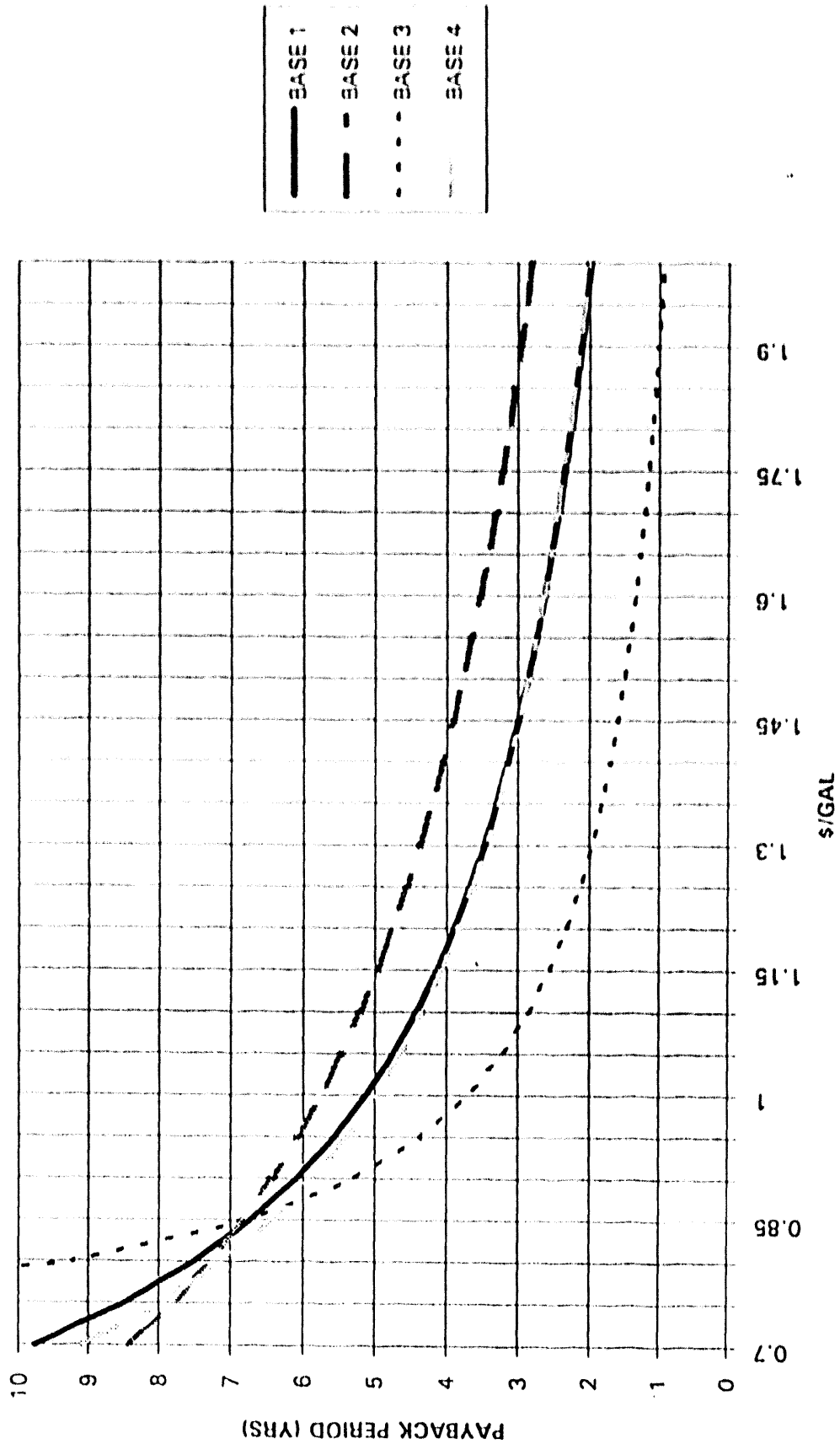


FIGURE 2.5

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

Alcohol Synthesis Loop

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

Summary

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

2.2.7 Application of Simulated Annealing for Optimisation of Chemical Process Flowsheet

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

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

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

2.2.6 Economic Analysis

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

Models

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

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

Potential Cost Reducing Methods For Coal Derived Alcohol Fuels

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

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

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

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

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

Alcohol Fuels Market

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

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

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

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

2.2.9 Fuels Evaluation

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

2.2.9.1 Blend Characteristics

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

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

On molar basis ;

$$\left[\frac{(1 - Y_M - Y_E - Y_P - Y_H)}{\bar{m}_I} \right] (C_{7.261}H_{13.87}) +$$

$$\left[\frac{Y_M V^* \rho_m}{\bar{m}_M} \right] C_4 H_9 OH + \left[\frac{Y_E V^* \rho_E}{\bar{m}_E} \right] C_2 H_5 OH +$$

$$\left[\frac{Y_P V^* \rho_P}{\bar{m}_P} \right] C_3 H_7 OH + \left[\frac{Y_H V^* \rho_H}{\bar{m}_H} \right] C_4 H_9 OH \rightarrow a CO_2 +$$

$$b H_2 O + CO_2 + d N_2$$

Where:

Y_I = volume fraction of indolene
 Y_M = volume fraction of methanol
 Y_{II} = volume fraction of ethanol
 Y_P = volume fraction of propanol
 Y_{II} = volume fraction of butanol

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

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

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

where

$$A = 1473.471 - 785.57065 y_M - 485.7355 y_{II} - 357.1806 y_P - 267.7698 y_{II}$$

$$B = 101.18082 + 5.80187 y_M + 8.24343 y_{II} + 7.3546 y_P + 7.18766 y_{II}$$

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

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

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

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

Possible alcohol (higher alcohols plus methanol) blends were determined based on the levels of fuel oxygen. This estimate is based on iso-butanol. By varying the volume percentages of C₁ - C₄ alcohols three blends with 5% and 10% wt. oxygen were chosen for the process synthesis work. Tables 2.5 and 2.6 given below give the volume ratios of the alcohols for a two-fuel oxygen levels required. Oxygen levels were selected based on the allowable limit that the existing vehicles can handle given their air/fuel ratio control technology. The two specific levels, 5% and 10% wt. oxygen were originally used by Douthit and Talbot (1983).

Table 2.5

Alcohol Blends with 10% (% vol.) Isobutanol

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

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

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

2.2.9.2 Engine

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

2.2.9.3 Combustion Characteristics

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

$$S_u = S_b - S_g$$

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

Where ;

S_b = flame speed

S_u = actual turbulent burning velocity

s_g = transport velocity

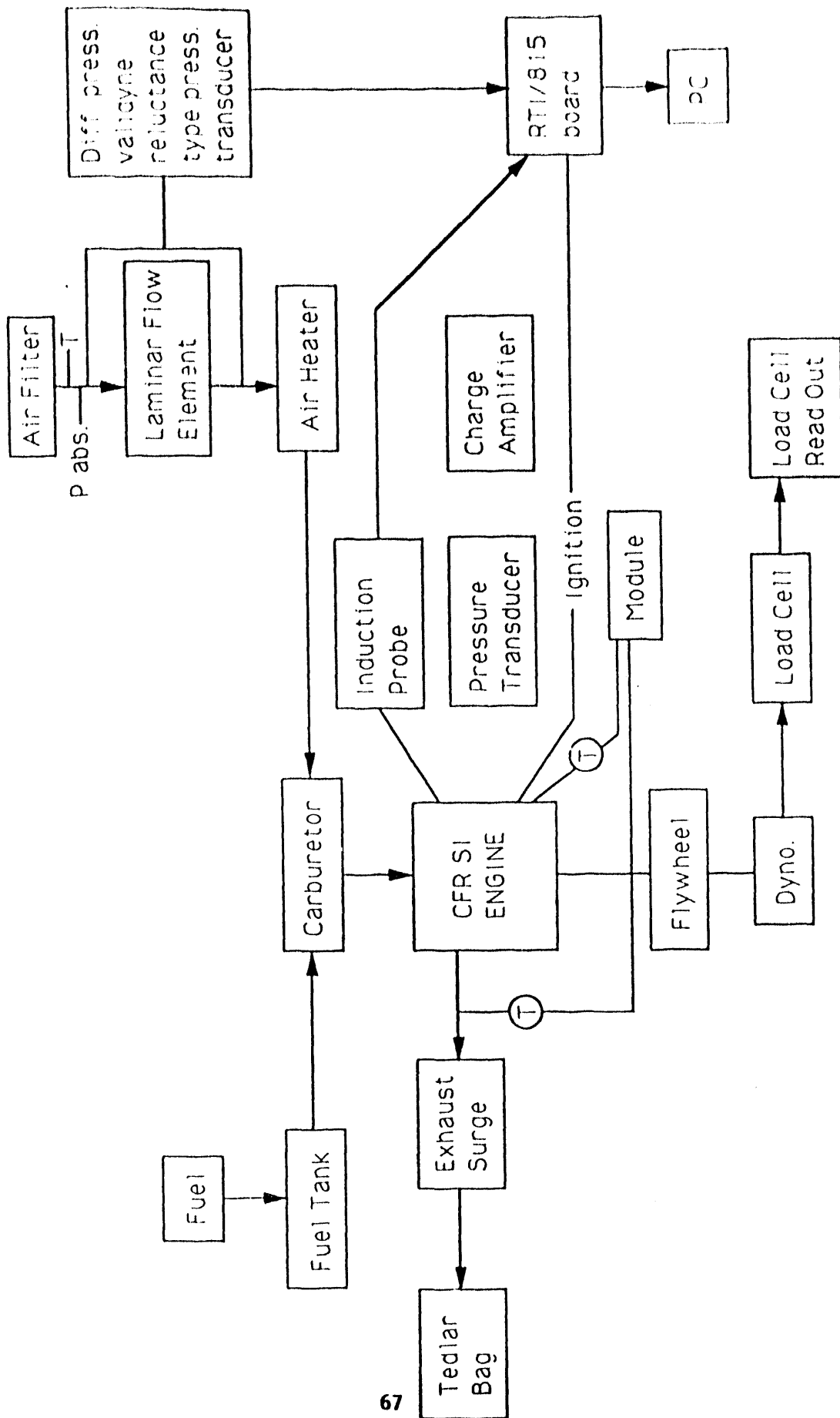
V_u = cylinder volume occupied by unburnt gas portion

V_t = total cylinder volume

A_f = frontal area

P = pressure

n = polytropic exponent



Layout of Instrumentation

FIGURE 2.6

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

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

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

where ;

k = global rate for all oxidation reactions

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

C_{pf} = specific heat at T_f

C_p = average specific heat at T_i and T_f

D_v = Diffusivity at T_v

E = activation energy

N_1 = moles of reactants

N_2 = moles of products

R = gas Constant

T_i = initial temperature

T_f = flame temperature

λ_v = thermal Conductivity at T_v

λ_f = thermal Conductivity at T_i

ρ_v = density at T_v

ρ_i = density at T_i

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

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

Where ;

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

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

$$K = x_1 K_1 + x_2 K_2$$

Where ; K , K_1 and K_2 = Reaction rate constants

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

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

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

2.2.9.4 Corrosion

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

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

2.3 Conclusions and Recommendations

2.4 Future Plans

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

2.5 Appendices for Task 2

2.5.1 Appendix 2-1

SYNGAS PRODUCTION FROM NATURAL GAS

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

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

COAL PREPARATION

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

Power needs = 1.9 MW

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

CRYOGENIC OXYGEN PLANT

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

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

Power needs = 0.0
Steam needs = 700 kg/hr, 1700 kPa, 250°C
Installed Capital Cost (1992 dollars) = \$76.7 MM

RECTISOL

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

Power needs = 1.0 MW
Steam needs = 1500 kg/hr, saturated, 200 kPa
11000 kg/hr, 350 kPa, 130°C
Installed Capital Cost (1992 dollars) = \$38.2 MM

TEXACO GASIFIER

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

Power needs = 0.5 MW
Steam needs = 6000 kg/hr, 350 kPa, 130°C
Installed Capital Cost (1992 dollars) = \$163.7 MM

SLAG HANDLING

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

estimated by exponential scaling.

Power needs = 0.0

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

COS HYDROLYSIS

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

SYNGAS HEAT RECOVERY

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

Heat removed = 4.44×10^8 kJ/hr

Power needs = 0.4 MW

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

CLAUS PLANT

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

Power needs = 0.2 MW

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

5000 kg/hr, 1700 kPa, 250°C

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

BEAVON PLANT

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

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

MOB, ALCOHOL SYNTHESIS LOOP

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

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

CO₂ REMOVAL

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

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

STEAM/POWER GENERATION

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

Power produced = 96 MW

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

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

COAL PREPARATION

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

Power needs = 5.2 MW

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

LURGI GASIFIER

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

Power needs = 1.3 MW

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

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

SLAG HANDLING

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

Power needs = 0.0

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

CRYOGENIC OXYGEN PLANT

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

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

Power needs = 0.0

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

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

COS HYDROLYSIS

The sulfide rich stream from the Rectisol Block (stream 25), a small stream of clean syngas (stream 38), and air (stream 39) are sent to the COS Hydrolysis Block where COS is converted to 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.

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 = 5.9 MW

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

60000 kg/hr, 350 kPa, 130°C

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

CLAUS PLANT

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

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

Power needs = 0.6 MW

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

11000 kg/hr, 1700 kPa, 530°F

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

BEAVON PLANT

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

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

MOS, ALCOHOL SYNTHESIS LOOP

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

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

CO₂ REMOVAL

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

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

STEAM/POWER GENERATION

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

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

Power needs = 209 MW

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

PRESSURE SWING ADSORPTION

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

Power needs = 0.1 MW

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

2.5.3 Appendix 2-3

SYNGAS PRODUCTION FROM NATURAL GAS

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

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

RECTISOL

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

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

PRESSURE SWING ADSORPTION

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

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

MoS₂ ALCOHOL SYNTHESIS LOOP

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

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

CO₂ REMOVAL

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

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

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

STEAM/POWER GENERATION

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

Power needs = 44 MW

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

2.5.4 Appendix 2-4

COAL PREPARATION

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

Power needs = 2.1 MW

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

TEXACO GASIFIER

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

Power needs = 0.5 MW

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

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

CRYOGENIC OXYGEN PLANT

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

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

Power needs = 0.0

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

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

RECTISOL

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

Power needs = 1.1 MW

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

11000 kg/hr, 350 kPa, 130°C

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

SLAG HANDLING

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

Power needs = 0.0

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

COS HYDROLYSIS

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

negligible.

SYNGAS HEAT RECOVERY

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

Power needs = 0.4 MW

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

CLAUS PLANT

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

Power needs = 0.3 MW

Steam needs = 6000 kg/hr, saturated, 4500 kPa
5000 kg/hr, 1700 kPa, 250 C

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

BEAVON PLANT

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

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

MoS₂ ALCOHOL SYNTHESIS LOOP

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

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

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

CO₂ REMOVAL

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

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

STEAM/POWER GENERATION

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

Power needs = 86.0 MW

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

SOUR GAS SHIFT CONVERTER

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

Installed Capital Cost = \$6.7 MM

2.6 References for Task 2

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. *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.
3. "Beavon Sulfur Removal Process," *Hydrocarbon Processing*, April 1984.
4. Frank, Marshall E. "Methanol: Emerging Uses, New Synthesis," *Chemtech*, June 1982.
5. Baasel, William D., *Preliminary Chemical Engineering Plant Design, 2nd edition*, Van Nostrand Reinhold, New York, 1990, pp.529-530.
6. T. Torries, personal communication
7. *Chemical Marketing Reporter*, August 31, 1992.
8. 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).
9. Kirkpatrick S., C.D. Gelatt Jr., and M.P. Vecchi. *Optimization by Simulated Annealing*, *Science*, **220**, 671, (1983)
10. 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).
11. Dingler, Janet, S. Nirula, W. Sedriks, Cost of Synthesis Gases and Methanol, SRI International, Menlo Park, Ca., February 1983.
12. Gibson, Thomas and T. Sasano, "Plasticizer Alcohols (C₄-C₁₃)," *Chemical Economics Handbook*, SRI International, Menlo Park, Ca., 1990.
13. Gibson, Thomas and T. Sasano, "Oxo Chemicals," *Chemical Economics Handbook*, SRI International, Menlo Park, Ca., 1990.
14. First Interim Report of the Interagency Commission on Alternative Motor Fuels, Unites States Alternative Fuels Council, September 30, 1990.

15. Szmant, H.H., *Organic Building Blocks of the Chemical Industry*, Wiley, NY., 1989.
16. Chaibongsai, S., (1980), "The Burning Velocity Inside a Spark-Ignition Engine with Different Turbulent Promoters", Ph.D. Dissertation, Wayne State University, DETroit, MI.
17. Douthit, W.H., and Talbot, A.F., (1983), "Assessment of Ether and Alcohol Fuels from Coal", USDOE Report, DE83-017589.
18. Metghalchi, M., and Keck, J.C., (1982), "Burning Velocities of Mixtures of Air with Methanol, Isooctane and Indolene at High Pressure and Temperature", Combustion and Flame, 48, pp. 191-2110, 1982.
19. Olikara, C. and Borman, G., (1975), "A Computer Program for Calculating Properties of Equilibrium Combustion Products with Some Applications to I.C. Engines", SAE 750468.
20. Patel, K.S., and Henein, N.A., (1986), "Effect of Blending Methanol and Indolene on the Burning Velocity and Performance in a CFR-S.I. Engine", SAE 860235.
21. Patel, K.S. and Henein, N.A., (1985), "Burning Velocities in Methanol-Indolene Air Mixtures in a CFR Engine", SAE 850111.
22. Schrock, M.D. and Clark, S.J., (1983), "Butanol-Acetone Blends as S.I. Engine Fuels", Transactions of the SAE, p. 723-727.
23. Miller, W.R. and R.A. Lang, "Great Plains Coal Gasification Plant Public Design Report," Volume 1, DOE/CH/10088-1874-Vol.1, July, 1985.