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

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Executive Summary

In Task 1, during this reporting period, we encountered and solved a problem in the analysis of the reaction products containing a small amount of heavy components. Subsequently, we continued with the major thrusts of the program. We analyzed the results from our preliminary studies on the packed-bed membrane reactor using the BASF methanol synthesis catalyst. We developed a quantitative model to describe the performance of the reactor. The effect of varying permeances and the effect of catalyst aging are being incorporated into the model. Secondly, we resumed our more-detailed parametric studies on selected non-sulfide Mo-based catalysts. Finally, we continue with the analysis of data from the kinetic study of a sulfided carbon-supported potassium-doped molybdenum-cobalt catalyst in the Rotoberty reactor.

We have completed catalyst screening at UCC. The complete characterization of selected catalysts has been started.

In Task 2, the fuel blends of alcohol and unleaded test gas 96 (UTG 96) have been made and tests have been completed. The testing includes knock resistance tests and emissions tests. Emissions tests were conducted when the engine was optimized for the particular blend being tested (i.e. where the engine produced the most power when running on the blend in question). The data shows that the presence of alcohol in the fuel increases the fuel's ability to resist knock. Because of this, when the engine was optimized for use with alcohol blends, the engine produced more power and lower emission rates.

Two papers are being prepared to present the results of some of the optimization work done by Task 2. The first paper is entitled "The Variation of Parameter Settings and Their Effects on Performance for the Simulated Annealing Algorithm." The focus of this paper is the simulated annealing algorithm that is being used to optimize the alcohol fuels facility. The second paper is tentatively titled "Optimization of a Large Scale Alcohol Fuels Blending Facility Using Simulated Annealing." The focus of this paper is to present the results of optimizations on the blending facility. The model and economics for this facility have been the primary focus of the work done by Task 2.

A portion of the Chemical Engineering Department Senior Class of 1996 was assigned the problem of finding a profitable use for the acid gas waste stream from Case 5 (Shell Gasifier, no natural gas). The constraints were that sulfuric acid was undesirable and producing sulfur for landfill was unacceptable. The resulting design appears to be a profitable process alternative to the traditional methods of acid gas desulfurization at the smallest scale coal to syngas to alcohol fuel process. It was assumed that approximately 10% of the market for products produced could be penetrated. The principal raw material purchased is ammonia which is reacted with SO_2 to produce ammonium sulfate. Natural gas reacts with H_2S to produce carbon disulfide (CS_2). Soda ash (Na_2CO_3) is reacted with SO_2 for production of sodium sulfite (Na_2SO_3) and sodium bisulfite ($NaHSO_3$).

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 separate subtasks: laboratory and equipment setup; catalysis research; and reaction engineering and modeling. Research at West Virginia University (WVU) is focused on molybdenum-based catalysts for higher alcohol synthesis (HAS). Parallel research carried out at Union Carbide Corporation (UCC) is focused on transition-metal-oxide catalysts.

1.2 Accomplishments, Results and Discussion

1.2.1 Laboratory Setup

During this reporting period, we modified the plug-flow reactor system used at WVU to test non-sulfide Mo-based catalysts. We immediately ran into problems in the analysis of reaction products containing a small amount of heavy components when non-sulfide Mo-based catalysts are used. Condensation was eliminated by modifying the injection port of the gas chromatograph (GC) to heat the carrier-gas line all the way to the columns, and also increased the temperature of the sampling valve. This worked, but led to loss of methanol during shakedown runs using the BASF catalyst. Accordingly, the temperature of the carrier-gas line and the sampling valve were modified to be below 150°C. Finally, we changed the injection sequence so that the sampling valve turns from the "load" position to the "inject" position only two minutes before injection. This allows a representative sample to be obtained but prevents accumulation of heavy products in the sampling loop between injections. Details can be found in MS57 and MS58.

1.2.2 Molybdenum-Based Catalyst Research

At WVU, we re-started our more-detailed parametric studies on selected non-sulfide catalysts. Currently in the plug-flow reactor is a Mo-Ni-K/C catalyst containing 18wt% Mo, with Ni/Mo = 0.6 and K/Mo = 1.2. We have carried out the reaction at 350°C and 750 psig, with different space velocities and different H_2/CO ratios. The effect of these parameters on overall reaction rate, methanol selectivity, higher-alcohol selectivity, and the production rate of alcohols upto hexanol have been described in MS58. The chain-growth probability parameter in the Anderson-Schultz-Flory representation has been shown to depend upon the H_2/CO ratio but not upon the overall space velocity.

We plan to carry out a three-variable design experiment on another of the selected catalysts, to obtain a kinetic model to describe its catalytic performance.

1.2.3 Transition-Metal-Oxide Catalyst Research

At UCC, screening runs have been completed. The catalysts have been sent for characterization. Some preliminary results have been received. Detailed analyses and comparisons of these results will be made when all the characterizations are available.

1.2.4 Reaction Engineering

The performance of the packed-bed membrane reactor is being evaluated using the BASF methanol-synthesis catalyst. A quantitative model has been developed incorporating a series of differential equations. Since there are four components, *viz.*, H_2, CO, N_2, CH_3OH, and since each is present on both the shell side and the tube side of the membrane, there are eight simultaneous differential equations to be solved. For example, in the tube side, the relation for hydrogen can be written as:

$$df_t/dz = -2(\Re RT_a/P_a)\pi r_1^2 \rho_b - 2\pi r_m(\mathcal{P}_{H2}RT_a/P_a)P_t(x_{H2} - y_{H2}) \quad (1)$$

Similar relations can be written for CO, N_2, and methanol. Analogously, on the shell side :

$$df_s/dz = 2\pi r_m(\mathcal{P}_{H2}RT_a/P_a)P_t(x_{H2} - y_{H2}) \quad (2)$$

In eqs (1) and (2), f_j is the volumetric flow rate of stream j (m^3STP/min); T_a, P_a are the standard temperature and pressure(25°C and 1atm); T_t, P_t are the reaction temperature and pressure (250°C and 750 psig); r_1 and r_m are the tube inner radius and log-mean radius; ρ_b is the density of the catalyst in the bed; x_i and y_i are the mole fractions of species i in the tube side and the shell side; $\Re$ is the rate of formation of methanol (in mol/min/kgcat) and $\mathcal{P}_i$ is the permeance of species i (in mol/min/m^2/Pa). Additional details of the model can be found in MS57.

The rate term $\Re$ was used only for the equations on the tube-side since the catalyst was not present on the shell side. The power-law rate form developed (as described in an earlier report) from the experiments on the fixed-bed reactor was used:

$$\Re = k\,(C_{CO})^a\,.(C_{H2})^b \qquad \text{mol/min/kgcat} \quad (3a)$$

where k is the rate constant, C_{CO} and C_{H2} are the concentrations of CO and H_2. Current best-fit values of the parameters k, a and b are:

$$k = 94500 \quad (3b)$$
$$a = 0.632 \quad (3c)$$
$$b = 1.147 \quad (3d)$$

We had carried out experiments previously for determining the permeances of three of the components (H_2, CO, and N_2), using the membrane reactor but without a catalyst and at the same experimental conditions as for the reaction. These values for $\mathcal{P}_i$ were used in the model. The values of permeances are (in mol/min/m^2/Pa):

$$\mathcal{P}_{H2} = 1.211 \times 10^{-7} \quad (4a)$$
$$\mathcal{P}_{CO} = 1.17 \times 10^{-7} \quad (4b)$$
$$\mathcal{P}_{N2} = 3.96 \times 10^{-7} \quad (4c)$$
$$\mathcal{P}_{MeoH} = 0.792 \times 10^{-7} \quad (4d)$$

The values of conversion at the exit of the membrane reactor can be obtained from the model equations (1) and (2), using the parameters in equations (3) and (4). Figure 1.1 shows the comparison between the values obtained

from the model and those observed experimentally after steady state at 250°C and 750 psig. Each flow condition number in Figure 1.1 represents a different feed rate of the reactants. The experimental conditions are given in Table 1.1. Flow condition 1 was taken with a fresh sample of catalyst and flow conditions 2 to 5 were taken with the same catalyst sample in the same order with time onstream. Flow condition 6 was taken with another fresh sample of catalyst and points 7 to 9 were taken with the same catalyst sample with time onstream. Table 1.1 indicates that at least one run at each flow condition was made at 250°C, but runs at 200°C and 225°C were made for most of the flow conditions. The order in which the runs were made at the various temperatures can be noted from the time range after the introduction of the catalyst in Table 1.1.

It can be seen from Figure 1.1 that the trend of the experimental data is the same as that obtained from the model. However, the values obtained from the model are higher than the actual experimental values. Further, the differences in the values are greater for flow conditions corresponding to later runs with the same sample of catalyst.

One probable reason for the error in the conversions obtained from the model and that observed in experiments is that the values of permeances $\mathcal{P}$ used might not be accurate. Therefore, an optimization procedure has been included. This procedure finds the values of the permeances of the four components so that the sum of the squares of the errors for the experimental data points is a minimum.

A second possibility is that the catalyst was not properly pretreated and may be subject to deactivation. We have introduced an exponential dependence of the rate constant on the time from introduction of the catalyst sample into the reactor. By fitting the data obtained at all temperatures and times from introduction at all flow conditions, we can obtain best-fit parameters for the pre-exponential factor, the activation energy and the deactivation constant at all flow conditions. This will allow us to obtain a value for the inital conversion at every flow condition. Preliminary values for these parameters have been obtained for flow conditions 1 and 6 at 250°C; see MS58.

These values can be used to obtain the best-fit values of the permeances $\mathcal{P}$ from the model above. In this manner, we will be able to compare the experimental and predicted values of the exit conversion from the packed-bed membrane reactor.

1.3 Conclusions and Recommendations

Reduced Mo-Ni-K/C materials continue to be considered as promising catalysts for HAS. The kinetic study using the Rotoberty reactor has been completed and analysis of the results is forthcoming. A model for the performance of a packed-bed membrane reactor in the synthesis of alcohols may be useful. Characterization of transition-metal catalysts used in HAS are forthcoming.

1.4 Future Plans

At WVU, work will resume on the detailed parametric studies on selected non-sulfide catalysts using the plug-flow reactor. The analysis of the packed-bed membrane reactor will continue.

UCC has completed catalyst screening. We plan to complete characterization of selected catalysts.

TABLE 1.1
FLOW CONDITIONS IN PACKED-BED MEMBRANE REACTOR RUNS
P_t = 750psig, NR = Not Run

FLOW CONDITIONS	CATALYST SAMPLE	FLOW RATE OF COMPONENT IN FEED STREAM (ml STP/min)					TIME RANGE AFTER CATALYST INTRODUCTION (h)		
		TUBE SIDE		SHELL SIDE			T = 250°C	T = 225°C	T = 200°C
		H_2	CO	H_2	CO	N_2			
1	A	50	50	0	0	40	0-22	22-36	36-54
2	A	50	50	0	0	60	54-66	NR	NR
3	A	50	50	0	0	100	66-82	82-96	96-108
4	A	40	40	0	0	40	120-134	108-120	134-146
5	A	40	40	0	10	40	158-172	146-158	NR
6	B	40	40	10	0	40	9-19	0-9	NR
7	B	40	40	10	10	40	19-29	29-38	NR
8	B	50	50	20	20	0	38-48	NR	NR
9	B	50	50	50	50	0	48-57	NR	NR

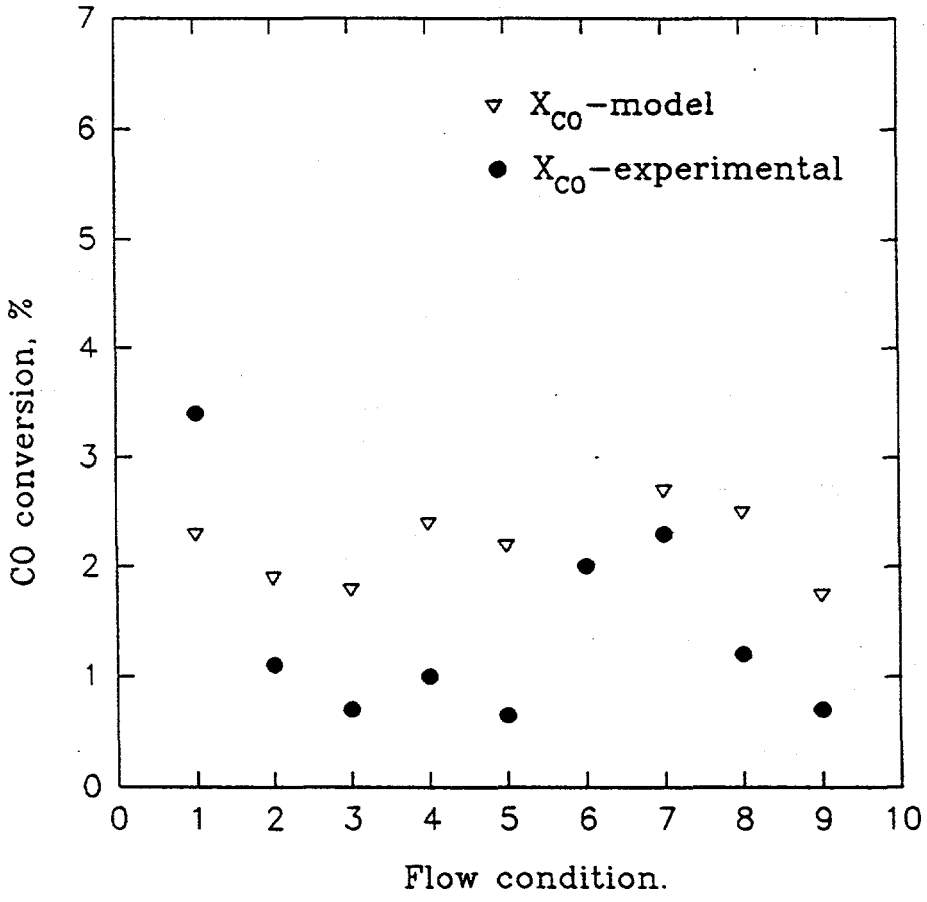

Figure 1.1 Comparison of experimental and model exit conversions from the packed-bed membrane reactor. Experimental values are steady-state values obtained at each of the flow conditions of Table I. Model values have been obtained by using the results of eqns (1)-(3) and the pre-calculated values of the permeances, eq (4).

2.1 Introduction

Internal combustion engine performance is strongly dependent on the type of fuel used in the engine. Engine performance parameters such as knock limiting compression ratio, power output, fuel consumption, and emissions are all functions of the fuel burned in the engine. The purpose of this research is to determine how engine performance will be affected by mixing various different alcohols with standard gasoline.

Six blends were selected for testing along with the baseline fuel, which is unleaded test gas 96 (UTG 96). The composition of the blends tested are given in Table 2.1 below.

Table 2.1 - Composition of the Blends Tested

	Percent Volume						
	UTG 96	Methanol	Ethanol	Propanol	Butanol	Pentanol	wt% Oxygen
Baseline	100.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Blend 1	90.00%	0.60%	2.07%	4.80%	2.40%	0.13%	3.03%
Blend 2	90.00%	0.60%	0.22%	4.80%	2.40%	1.98%	2.72%
Blend 3	90.00%	2.00%	2.00%	3.00%	2.88%	0.12%	3.34%
Blend 4	90.00%	2.00%	2.00%	3.00%	0.12%	2.88%	3.24%
Blend 5	90.00%	3.24%	2.40%	2.76%	0.13%	1.47%	3.70%
Blend 6	90.00%	3.04%	2.40%	2.96%	1.47%	0.13%	3.70%

The tests were performed using a single cylinder Waukesha Fuel Research Engine which has been fitted with appropriate instrumentation. The most important instrumentation equipment include the pressure measurement inside the combustion chamber and the emissions sampling system, both of which have been described throughout the course of this project.

Two papers are being prepared to present the results of some of the work done by WVU Task 2. These results are from work that as been completed over the last two years. The first paper is entitled "The Variation of Parameter Settings and Their Effects on Performance for the Simulated Annealing Algorithm." The focus of this paper is the simulated annealing algorithm that is being used to optimize the alcohol fuels facility, which is the primary goal of Task 2. This paper has been through two drafts and we will submit it to the journal *Computers and Chemical Engineering* by the end of August. An extended abstract of this paper is included below. The second paper is tentatively titled "Optimization of a Large Scale Alcohol Fuels Blending Facility Using Simulated Annealing." The focus of this paper is to present the results of our optimizations on the blending facility. The model and economics for this facility have been the primary focus of the work done by WVU Task 2. The first draft of this paper is expected to be completed by the middle of July, and we will submit it to the journal *Industrial and Engineering Chemistry Research* by the end of August. An abstract of this paper is also included below.

A portion of the Chemical Engineering Department Senior Class of 1996 was assigned the problem of finding a profitable use for the acid gas waste stream from Case 5 (Shell Gasifier, no natural gas). The constraints were that sulfuric acid was undesirable and producing sulfur for landfill was unacceptable. The resulting design appears to be a profitable process alternative to the traditional methods of acid gas desulfurization at the smallest scale coal to syngas to alcohol fuel process.

2.2 Accomplishments, Results, and Discussion

2.2.1 Fuel Testing

Tests were conducted to determine the knock limiting compression ratio of each blend. Knock limiting compression ratio is a function of the spark timing, therefore, a knock limiting compression ratio was found for spark timings between 30° before top dead center (BTDC) and 5° BTDC in 2.5° increments. The knock limit was found by analyzing pressure histories inside the combustion chamber using a third derivative knock detection method outlined by Checkel and Dale [1]. In addition, the indicated mean effective pressure, which is a measure of engine power output, was calculated at the knock limit points. These results are presented in Figures 2.1 though 2.7. These figures show the knock limiting compression ratio (KLCR) for each spark timing and the corresponding indicated mean effective pressure (IMEP).

To get a feel for the difference in the resistance to knock between blends, the knock limit curves were numerically integrated over the spark timing range. These results are given in Figure 2.8. From observation of this data, it can be seen that the more lower alcohols there are in the blend (thus the more oxygen by weight in the blend), the higher the blend's resistance to knock. Blends 5 and 6 showed the best resistance to knock, and they had the maximum amount of oxygen by weight allowed by the DuPont Waiver (3.70%). Blends 1 and 3 were both below blends 5 and 6 but above blends 2 and 4 in knock resistance capability. All of the blends tested showed much higher knock resistance than clear gasoline.

As mentioned earlier, the IMEP for each knock limit point was calculated from the pressure history inside the combustion chamber. The purpose for this was to find the point where the engine produced the most power. The emissions tests were performed at this combination of spark timing and compression ratio which produced the most power from the engine. Further, the emissions tests were all conducted at a stoichiometric air to fuel ratio for the blend being tested. Emissions data reported are CO, CO_2, NO_x, and Organic Matter Hydrocarbon Equivalent (OMHCE). The data is reported in mass per unit time per unit power output (g/BHP-hr). The OMHCE is a measure of the total hydrocarbons emitted from the engine and takes into account unburned gasoline, unburned alcohol, and partially burned alcohol. Further, OMHCE is a quantity used by the EPA and is outlined in the Code of Federal Regulations [2].

Emissions data are presented in Figures 2.9-2.13. Figure 2.9 shows power output comparison between blends at the optimum spark timing/compression ratio combination for each blend. Clearly, Figure 2.9 shows that all of the blends produced more power than did clear gasoline. Further, the emission rate per unit power per unit time is less for each blend when compared to clear gasoline, with the CO_2 emissions being the most drastic.

2.2.2 Optimization

The optimization work is nearing completion. Two papers are being prepared to present the results of some of the work done by WVU Task 2. The focus of the first paper is the simulated annealing algorithm that is being used to optimize the alcohol fuels facility. The focus of the second paper is to present the results of our optimizations on the blending facility. These abstracts are included below.

2.2.2.1 Abstract of Paper on Simulated Annealing Optimization Algorithm

We present a simulated annealing algorithm using six parameters. These parameters are : IP, which is the *a priori* probability of the first attempted move of the optimization being accepted; N, which is the number of move attempts made during each temperature level; **a**, which is the rate of decrease of the temperature for each temperature level; **l**, which controls the maximum distance through the system space for a move attempt; **w**, which controls the rate of decrease of the maximum attempted move length with respect to the current temperature; and **k**, which describes the minimum variation in the objective function during the optimization before the algorithm is terminated. Using both Haverly's Pooling Problems and a Benzene Alkylation Problem, we have studied the effect that varying the values of these parameters has on the performance of the annealing algorithm. These problems have been transformed such that all variables have the same range and all constraints have been eliminated except those that define this range. The result of these transformations is that we have standardized the problems we are solving in order to make comparisons between the optimal simulated annealing parameters for the different problems being studied. We have compared the results obtained by using both single variable system state changes and multiple variable system state changes. We have found that for our transformed problems, and perhaps because of the transformations, single variable system state changes yield superior annealing results. For the two problems studied, we have shown that the best values for all parameters except **l** are largely problem independent. The accompanying figure shows a sample of the results we have obtained.

2.2.2.2 Application to Alcohol Fuel Blending Facility

We present the results of an optimization on a large scale alcohol fuels blending facility. This facility is comprised of four distinct process sections, each with its own economics and process variables. First is the coal gasification section, with many individual process blocks. The economics of each of these blocks are considered to be functions of the process flow rates. The alcohol synthesis section uses estimates of product outputs as functions of the reactor conversion. The output of the alcohol synthesis section is sent to the separations section, which is a complex series of distillation columns. Any or all of these columns may be used or by-passed. The individual alcohol streams from the distillation section are then mixed with gasoline components to make oxygenated fuels in the blending section. Because all of the constraints in the blending section are linear, we are able to use a linear optimization routine to solve for the optimal blending configuration during each pass of the simulated annealing algorithm. We have used simulated annealing to optimize this complex network of processes in order to determine the economic feasibility of the proposed facility.

2.2.3 Analysis of Acid Gas Waste Stream

A portion of the Chemical Engineering Department Senior Class of 1996 was assigned the problem of finding a profitable use for the acid gas waste stream from Case 5 (Shell Gasifier, no natural gas). The constraints were that sulfuric acid was undesirable and producing sulfur for landfill was unacceptable.

The student design group investigated the possibility of producing specialty sulfur chemicals from an acid gas waste stream produced by a coal gasification facility. In this facility, a Shell gasifier is used to process approximately 16,000 tons of coal per day into a synthesis gas used primarily to produce higher alcohol oxygenates and fuel additives. The process produces a waste gas stream of 50,000 kg/hr with the following composition:

Carbon Dioxide	62.07 mol %
Hydrogen Sulfide	33.18 mol %
Carbonyl Sulfide	3.34 mol %
Ammonia	0.81 mol %
Methanol	0.56 mol %

The usual method for the treatment of a waste gas of this type is a sequential application of the Claus and Beavon processes, resulting in elemental sulfur suitable for landfill. It was suggested that the students explore the possibility of producing sulfur chemicals from the stream. It was further indicated that they should avoid bulk chemicals such as sulfuric acid. Accordingly, the students began a review of the market for sulfur chemicals in an attempt to identify likely candidates for production. The sheer bulk of the raw material stream (50 metric tons/hr) required that the products have a considerable market, assuming that a new process would enter at approximately 10% of any product market. This requirement aided in narrowing the search from an initial 300 compounds to approximately 15 likely candidates for production. This was the first step in a feasibility study which was completed in December 1995. The feasibility study described two profitable options for the production of a variety of products. One option was based on desulfurization of the acid gas stream via a Claus Unit, then further processing of the elemental sulfur into value added products such as phosphorus pentasulfide and sodium hydrosulfide. The other option involved separation of the H_2S from the gas stream and production of SO_2, then further processing of these gases into carbon disulfide, ammonium sulfate, sodium sulfite and sodium bisulfite. The students were assigned the latter option, and Phase II of the Sulfur Project (the design phase) began in January 1996.

The final product is the completed Sulfur Project Design. The design consists of six individual Units, with Units 200, 300, and 400 producing the compounds listed above, in addition to byproduct hydrogen in Unit 200. Unit 100 performs the initial separation of H_2S from the acid gas waste stream. Unit 500 combusts a portion of this H_2S to produce SO_2, which is the principal feedstock for Units 300 and 400. The heat generated by this combustion supplies steam for heating to Units 100 and 200. Waste gases are generated in Units 100, 300, and 400 which require treatment. Unit 600 is a scrubber facility which reduces the pollutants in these waste gas streams to permissible levels.

This process is a profitable alternative to the traditional methods of acid gas desulfurization which involve production of elemental sulfur and, less commonly, sulfuric acid. Sulfur emission regulations have become increasingly stringent. This has had the effect of oversupplying the market for elemental sulfur, which has depressed the value and has led some producers to landfill sulfur which they could not sell. The markets for the products produced by this process are large and have historically exhibited stability in both price and market size. The raw material requirements for the process are few and relatively inexpensive compared to the products. The principal raw material purchased is ammonia which is reacted in Unit 300 with SO_2 to produce ammonium sulfate. Unit 200 uses pipeline supplied natural gas to produce carbon disulfide. Unit 400 requires a supply of soda ash for production of sodium sulfite and bisulfite. Lesser amounts of process water and solvents are purchased for the various Units, but these costs are not significant. Utility requirements are similarly low since the great majority of heating is accomplished with steam supplied from Unit 500.

The total Fixed Capital Investment (FCI) for the process is approximately $54 million. The total cost of manufacturing, including raw materials, labor, and utilities amounts to $44 million yearly. Product revenues are in the $80 million / yr range, giving an after-tax net present value (NPV) of $79 million. This assumes a tax rate of

42%, a ten-year operating life, and an internal rate of return of 9%. The calculation was performed assuming a two-year construction phase, with the total capital investment split evenly over the two years. Working capital was assumed to be 20% of the total fixed capital investment. The payoff period (discounted) is four years.

Due to time constraints, the students did not do a detailed design of Units 300 and 400. In order to evaluate the entire process, however, capital and operating cost estimates were prepared for these Units based on the number and types of equipment required, the capacities, and estimated raw material and energy requirements.

2.3 Conclusions

The results of fuel testing show that an engine will produce more power when run on a blend of gasoline and alcohol when the engine is optimized for the particular fuel. This is because the presence of alcohol in the fuel allows the compression ratio to be increased past the maximum point that can be run with clear gasoline. This increased power output also causes the emission rate to be lower. The problem with optimizing engines in the market for use with gasoline/alcohol blends is the fact that gasoline/alcohol blends would have to be available everywhere, and right now they are not. An engine optimized to be run on a blend would not run correctly if the engine was fueled with clear gasoline.

Another conclusion from this research is that the lower alcohols (methanol, ethanol, propanol) seem to increase the ability of the fuel blend to resist knock more than the higher alcohols (butanol, pentanol). The problem with using higher concentrations of the lower alcohols is that the oxygen content in the blend by weight goes up.

Two papers are being prepared to present the results of the optimization work. One paper involves the simulated annealing algorithm that is being used to optimize the alcohol fuels facility, The other involves the results of optimizations on the alcohol fuel blending facility.

The problem of finding a profitable use for the acid gas waste stream from Case 5 (Shell Gasifier, no natural gas) was investigated. The constraints were that sulfuric acid was undesirable and producing sulfur for landfill was unacceptable. It was assumed that approximately 10% of the market for products produced could be penetrated. The resulting design appears to be a profitable process alternative to the traditional methods of acid gas desulfurization at the smallest scale coal to syngas to alcohol fuel process.

2.4 Future Work

Plans for future research in fuel testing include comparing ignition delay times and burn times between the blends and the baseline fuel. In addition, the fuels will be sent to an outside lab for research octane, motor octane, reid vapor pressure, and distillation tests. This should be completed before the end of July and the results will be reported in the July monthly report.

2.5 Bibliography

1. M. D. Check and J. D. Dale, "Computerized Knock Detection from Engine Pressure Records," Society of Automotive Engineers Paper 860028, 1986.

2. National Archives and Records Administration. Code of Federal Regulations 40, Protection of the Environment. Revised as of July 1, 1994.

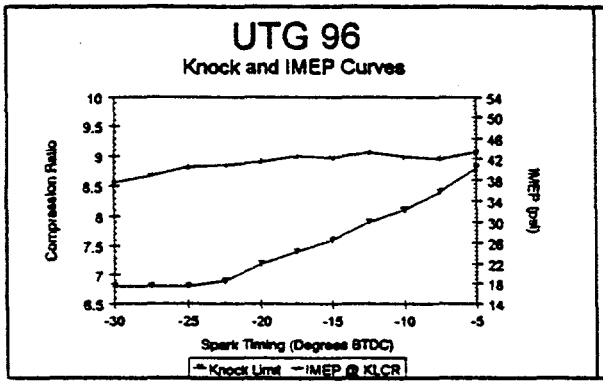

Figure 2.1 - Unleaded Test Gas 96 Knock Limit and IMEP Curves

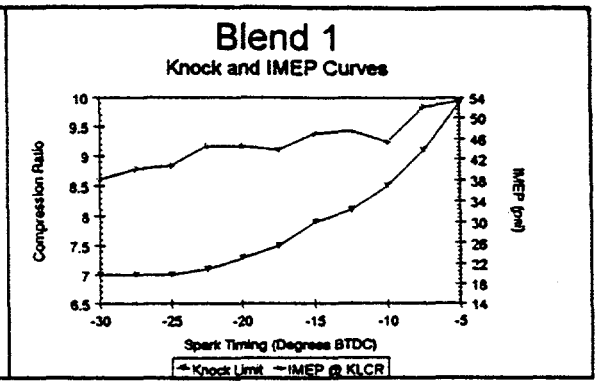

Figure 2.2 - Blend 1 Knock Limit and IMEP Curves

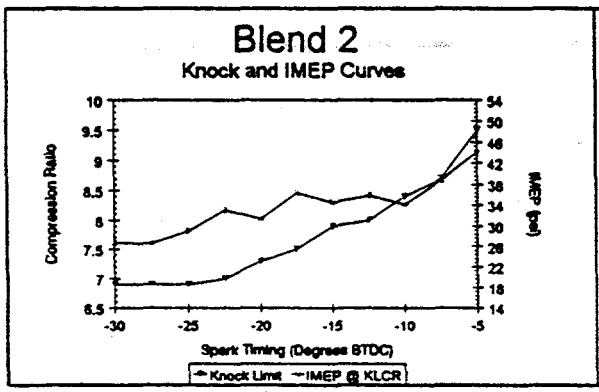

Figure 2.3 - Blend 2 Knock Limit and IMEP Curves

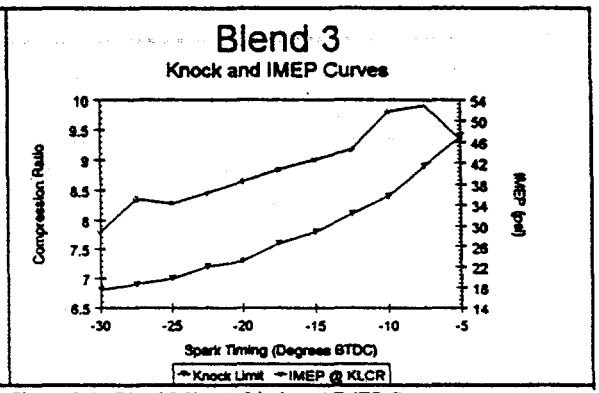

Figure 2.4 - Blend 3 Knock Limit and IMEP Curves

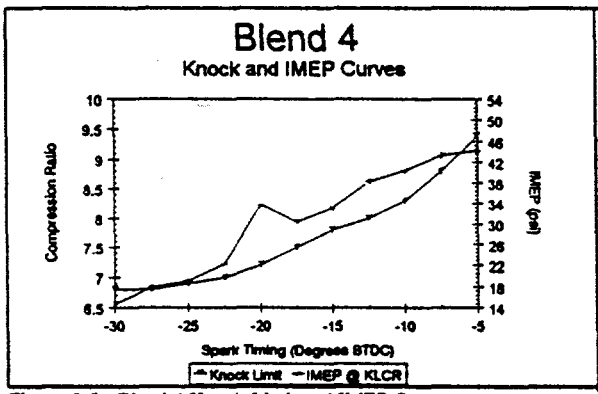

Figure 2.5 - Blend 4 Knock Limit and IMEP Curves

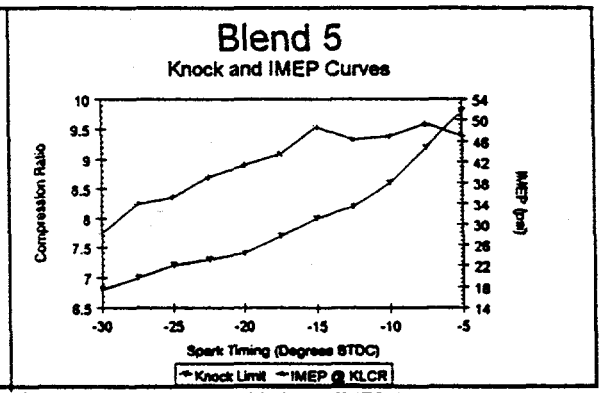

Figure 2.6 - Blend 5 Knock Limit and IMEP Curves

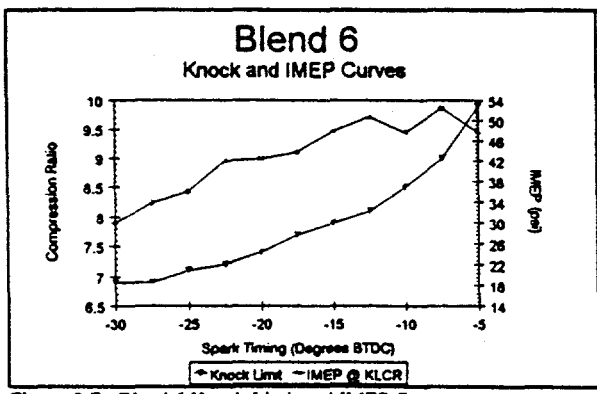

Figure 2.7 - Blend 6 Knock Limit and IMEP Curves

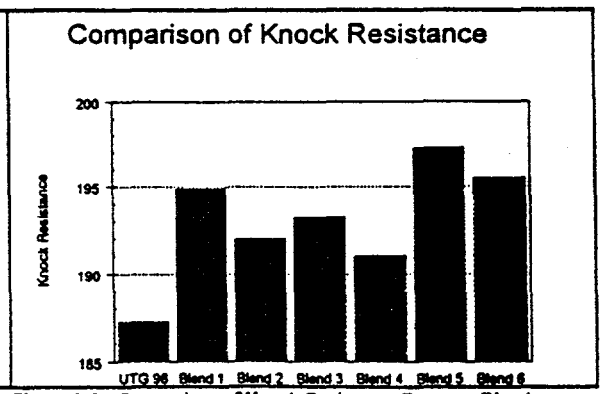

Figure 2.8 - Comparison of Knock Resistance Between Blends

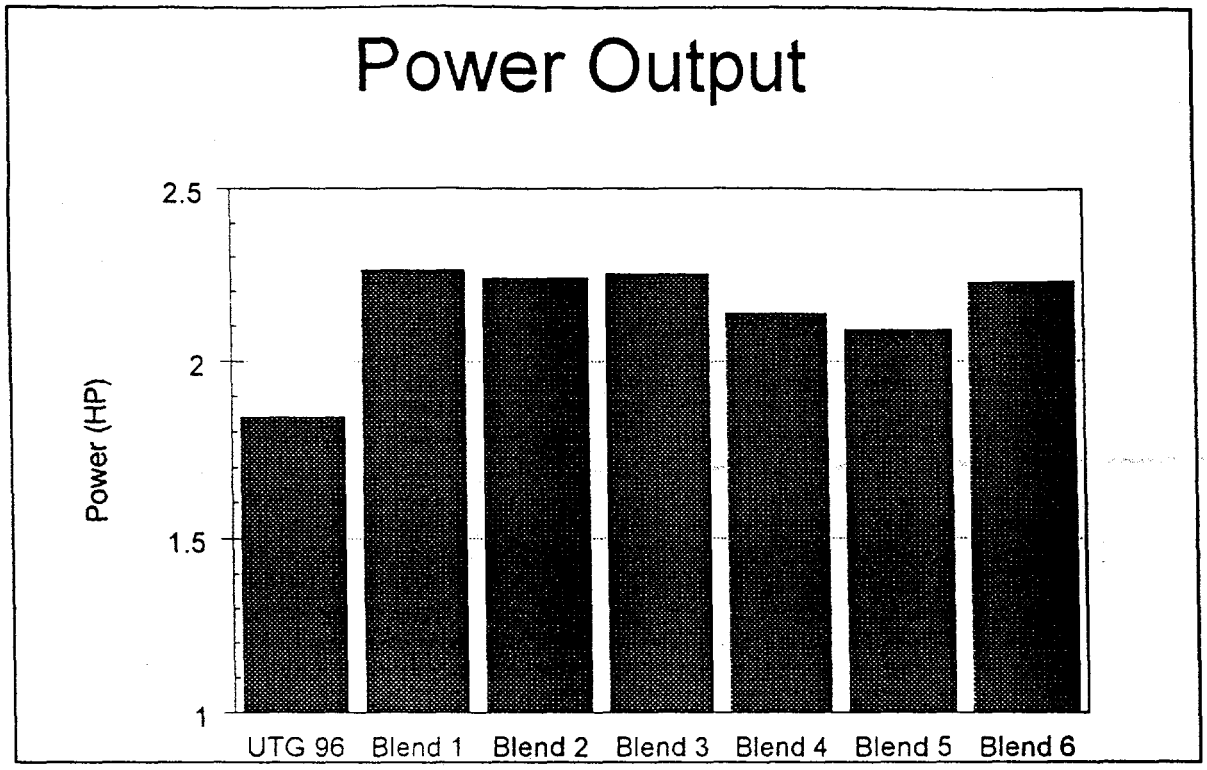

Figure 2.9 - Comparison of Power Output Between Blends at their Best Setpoints

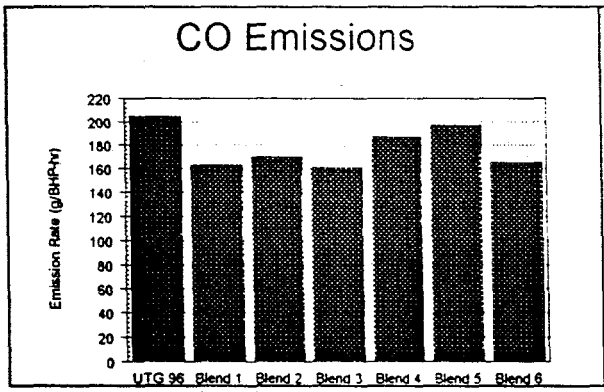

Figure 2.10 - Comparison of CO Emissions Between Blends

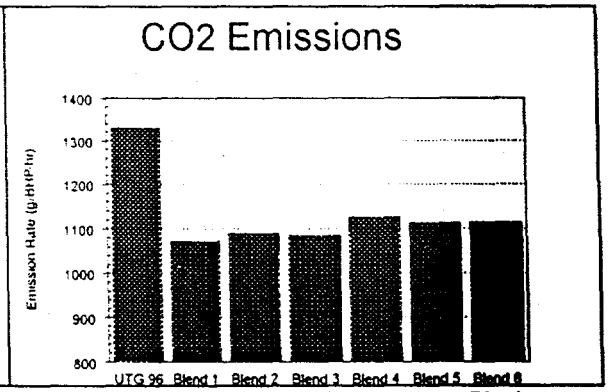

Figure 2.11 - Comparison of CO_2 Emissions Between Blends

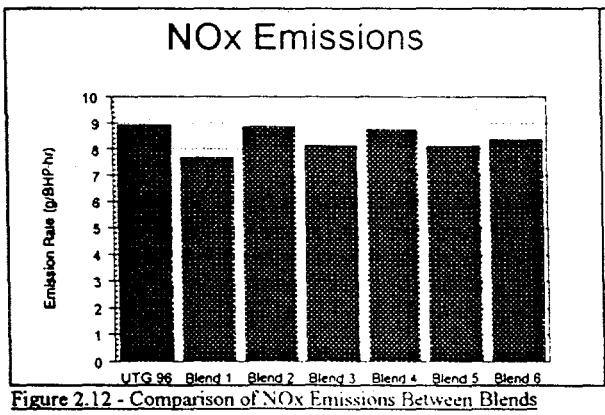

Figure 2.12 - Comparison of NOx Emissions Between Blends

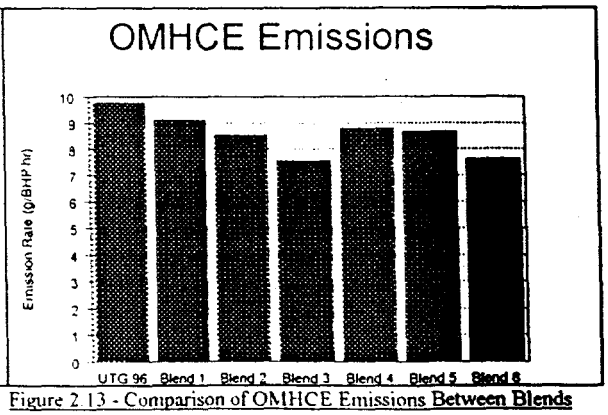

Figure 2.13 - Comparison of OMHCE Emissions Between Blends

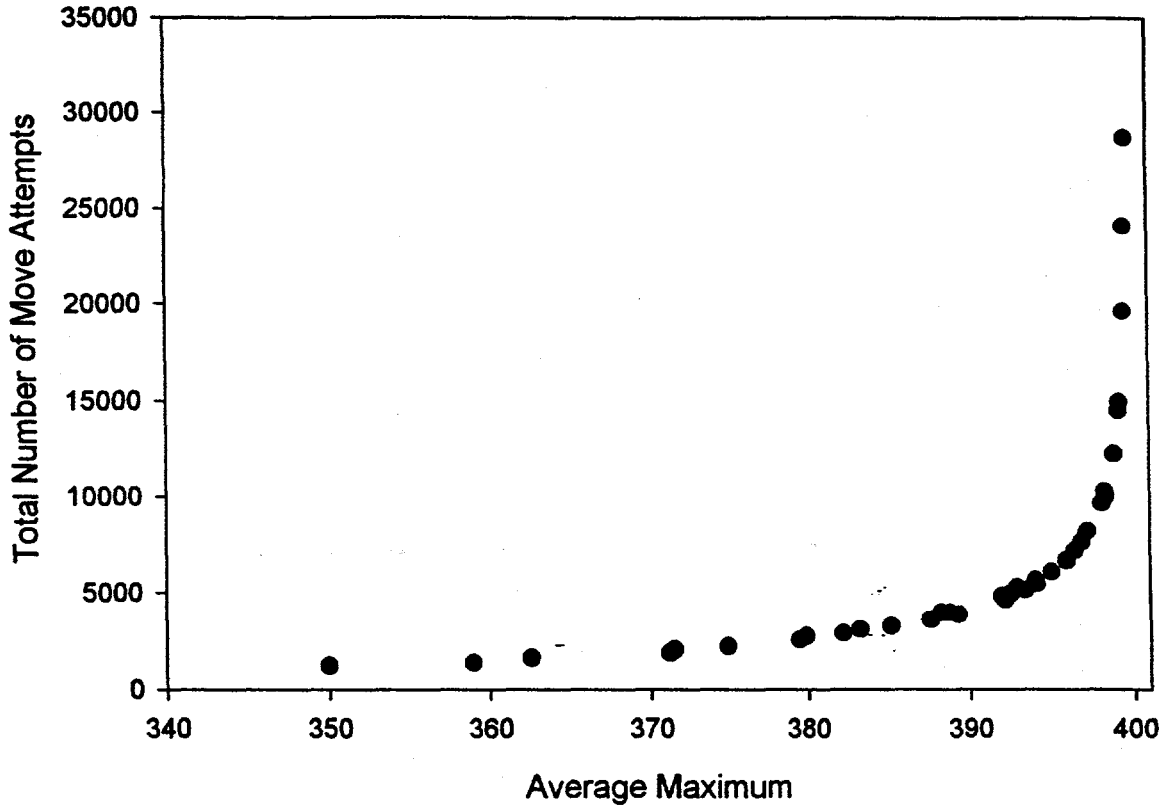

Figure 2.14a: Correlation Between Average Maximum and Total Number of Move Attempts for Haverly's Pooling Problem I

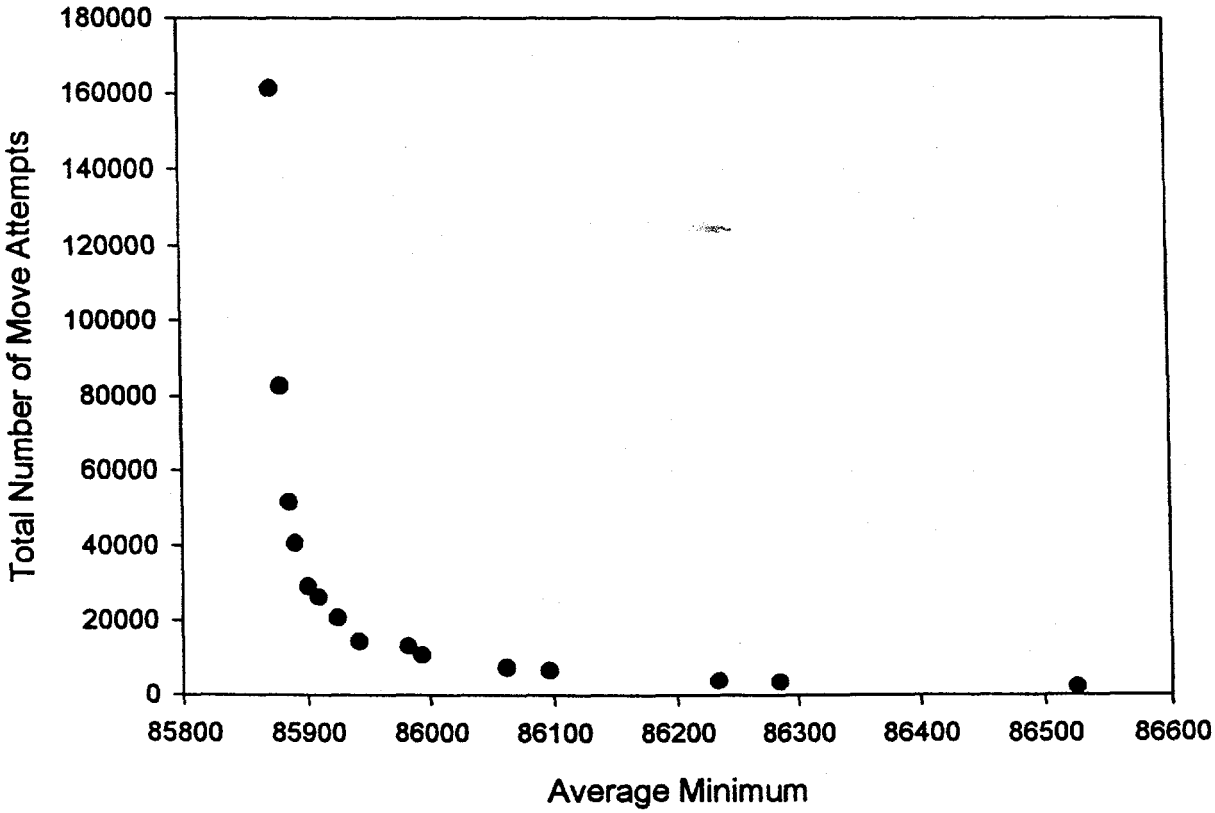

Figure 2.14b: Correlation Between Average Minimum and Total Number of Move Attempts for Modified Benzene Alkylation Problem

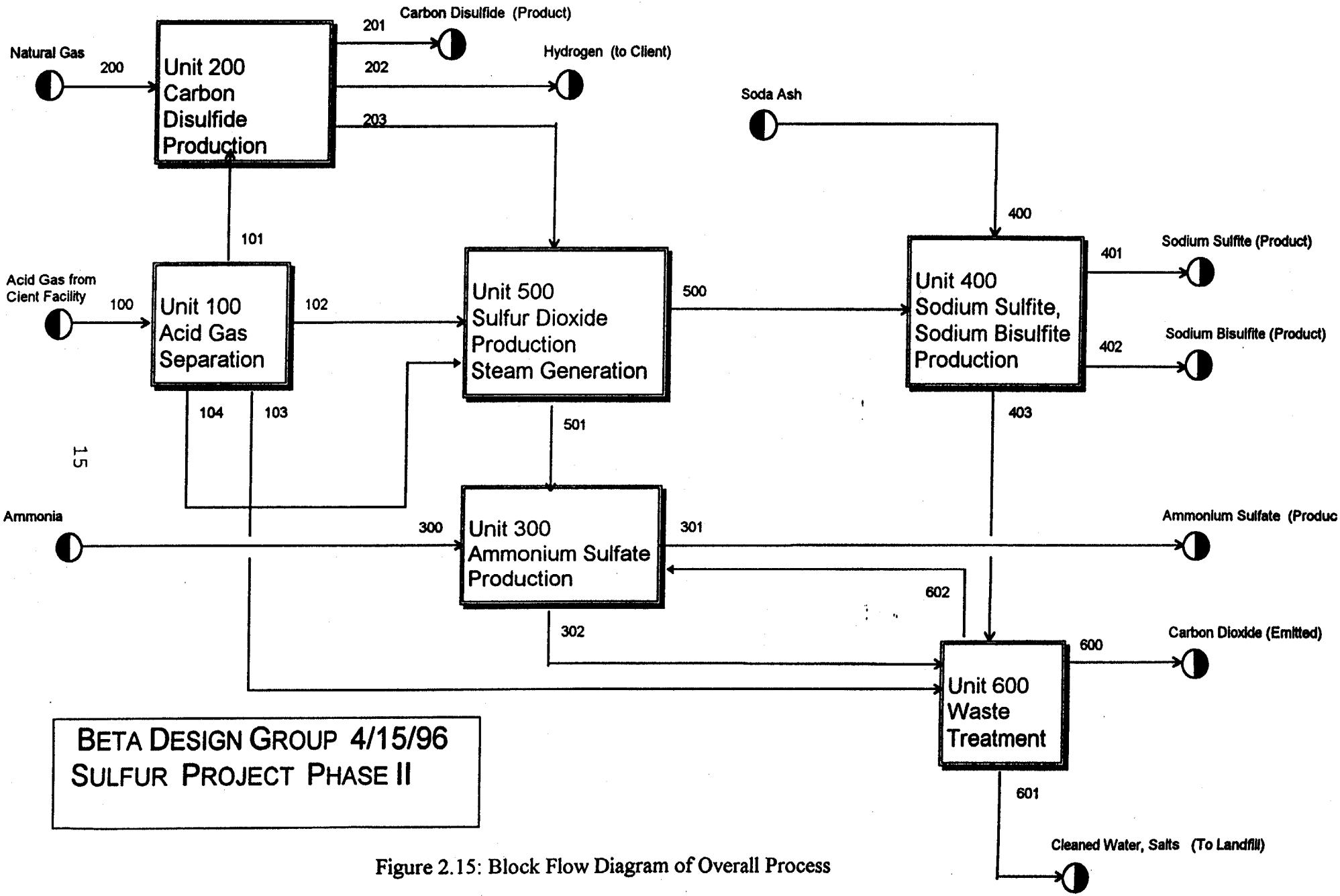

Figure 2.15: Block Flow Diagram of Overall Process