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

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

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Executive Summary

Task 1; During this reporting period, there were three major thrusts in the WVU portion. First, we started a preliminary investigation on the use of a membrane reactor for HAS. Accordingly, the plug-flow reactor which had been isolated from sulfides was substituted by a membrane reactor. The tubular membrane was first characterized in terms of its permeation properties, *i.e.*, the fluxes, permeances and selectivities of the components. After that, a BASF methanol-synthesis catalyst was tested under different conditions on the membrane reactor. The results will be compared with those from a non-permeable stainless steel tubular reactor under the same conditions. Second, we started a detailed study of one of the catalysts tested during the screening runs. Accordingly, a carbon-supported potassium-doped molybdenum-cobalt catalyst was selected to be run in the Rotoberty reactor. Finally, we have started detailed analyses of reaction products from some earlier screening runs in which non-sulfide molybdenum-based catalysts were employed and much more complicated product distributions were generally observed. These products could not hitherto be analyzed using the gas chromatograph which was then available. A Varian gas chromatograph/mass spectrometer (GC/MS) is being used to characterize these liquid products.

At UCC, we completed a screening of an Engelhard support impregnated with copper and cesium. We have met or exceeded three of four catalyst development targets. Oxygenate selectivity is our main hurdle. Further, we tested the effect of replacing stainless-steel reactor preheater tubing and fittings with titanium ones. We had hoped to reduce the yield of hydrocarbons which may have been produced at high temperatures due to Fischer-Tropsch catalysis with the iron and nickel in the preheater tube walls. Results showed that total hydrocarbon space time yield was actually increased with the titanium preheater, while total alcohol space time yield was not significantly affected.

A poster paper entitled "Modeling and Simulation of a Packed-Bed Membrane Reactor for Improved Production of Higher Alcohols from Synthesis Gas" by A. Subramanian, R. Y. K. Yang, D. B. Dadyburjor, and E. L. Kugler was presented by Ray Yang at the AIChE Annual Meeting during November 12-17, 1995. In addition, all facets of this task were presented and discussed at the DOE Program Review held at WVU on December 15, 1995.

Task 2; in fuel testing, emissions from different alcohol blends have been measured and both blends show a decrease in the CO emissions compared to the baseline. Additionally, both alcohol blends show a reduction in the Total Hydrocarbons (THC) emissions (~ 10%) compared to that of the baseline. Finally, both blends show a reduced peak of NO_x emissions and reduced CO_2 emissions compared to that of the baseline.

A Monte Carlo uncertainty study on the manufacturing cost was performed using the hybrid Shell/Natural Gas Case. The results show that there is approximately 10% chance of meeting the benchmark return. From the data generated in the uncertainty analysis simulations, sensitivity analyses were performed to determine which uncertain inputs had the greatest effect on the manufacturing cost. The Shell gasifier capital cost, the electrical power credit, and the coal cost were significantly more important on this basis than were the other costs.

For the alcohol fuel blending facility, we have used preliminary data to obtain some results for the optimization problem. In the direction of increasing gasoline flow, we notice an initial drop in the profitability, followed by increasing profitability until it levels off and remains constant. This is expected because the blending value of the alcohol product is currently less than the manufacturing cost.

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, the plug-flow reactor which had been isolated from sulfides was converted to a membrane reactor in order to explore and to evaluate new reactor concepts that could be used for HAS synthesis. The schematic configuration of this reactor system can be found in MS50. Two GCs are used for analysis of products: one for sweep side and the other for the whole mixture. Argon is used as carrier gas for both GCs, so as to analyze H_2, CO, N_2, CO_2, H_2O and any other products at the same time. Response factors for H_2, CO and N_2 in both GCs were determined by varying the pressure of each individual gas and obtaining the area in each GC.

In the other reactor setup, because of the large volume of the Berty reactor, the ranges of the mass flow controllers for CO and H_2 were increased. The new values are 500 cc/min and 1000 cc/min, respectively. The scaled-up values allow us to obtain higher flow rates so as to maintain a residence time comparable with the plug-flow reactor and to stabilize the reaction more quickly. However, the available feed gas was depleted rapidly. Consequently, this set-up was non-functional for about two months.

As mentioned in previous reports, we could not conclusively identify many products when non-sulfide molybdenum based catalysts were used earlier. To identify these products, a GC/MS was purchased and is being used to analyze the liquid products from selected past runs. Chemical ionization has been used, with CH_4 as the ionization gas. A library was constructed in our laboratory from oxygenate and hydrocarbon standards. We can now identify conclusively most of the major GC peaks that were previously unidentifiable.

1.2.2 Molybdenum-Based Catalyst Research

From the catalysts screened to date, a carbon-supported potassium-doped molybdenum-cobalt catalyst was selected for a more-detailed study of the kinetics. A sample of this catalyst was placed in the Berty reactor. Preliminary results showed that it takes a long time for the reaction to reach steady state. Some results can be seen in MS50. Work with this reactor set-up had to be pushed back because of problems with the delivery of feed gas.

Due to the unavailability of the Berty reactor setup, we started preliminary studies on the membrane reactor. The permeation properties of this reactor were first characterized by feeding H_2 and CO in various compositions on the tube side of the reactor, and N_2 on the sweep side of the reactor. The fluxes, permeances and selectivities of the components determined at varying N_2 sweep rates and reactor temperatures were calculated, and are listed in MS51. The permeance and flux of each gas decreases with increasing temperature. The permeance and flux of tube-side gas increases with increasing sweep flow rate and the increase is significant. The permeance of H_2 does not increase very much with increase in the inlet concentration, but that of CO does increase significantly with increase in the inlet concentration. The selectivity of H_2 over CO is below that expected under a Knudsen diffusion regime.

The membrane reactor was then tested with the BASF methanol-synthesis catalyst used earlier for checking out the other reactors. The results indicate that the conversion is very sensitive to even small changes in the sweep flow rate. Lower sweep flow rates give higher conversions. Contrary to what we would expect for a conventional plug-flow reactor, the effect of increasing residence time of the reactants inside the membrane tube is to reduce the CO conversion, probably due to increase in the loss of unreacted reactants. Furthermore, the introduction of reactants, instead of an inert, on the sweep side, increases the conversion. Also, at lower sweep flow rates, the loss of unreacted reactants plays a dominant role; whereas at higher sweep flow rates, the dilution of the reactants inside the tube is the key point. These results will be compared with those from a non-permeable stainless-steel tubular reactor.

In this regard, a poster paper, "Modeling and Simulation of a Packed-Bed Membrane Reactor for Improved Production of Higher Alcohols from Synthesis Gas" by A. Subramanian, R. Y. K. Yang, D. B. Dadyburjor, and E. L. Kugler, was presented by Ray Yang at the AIChE Annual Meeting during November 12-17, 1995.

Currently, GC/MS is being used to analyze the liquid products collected from selected past runs when non-sulfide molybdenum-based catalysts were employed. By tracing back to the original GC spectra, we have shown that a series of reduced Mo-Ni-K/C catalysts is very promising. The original experimental runs, carried out at 350°C, 750 psig, GHSV of 6000 l/kg catalyst/h and $H_2/CO=1$, have now been shown to result in alcohol production rates as high as 350 g/kg catalyst/h and a CO_2-free selectivity of more than 50% by weight to higher alcohols. We expect to carry out some parametric and kinetic studies for this series of catalysts in the future.

A summary of this work was presented and discussed at the DOE Program Review held at WVU on December 15, 1995.

1.2.3 Transition-Metal-Oxide Catalyst Research

At UCC, we completed experiments using an Engelhard support impregnated with copper and cesium. Copper concentration was varied while cesium concentration was kept constant at 5.0 pph. We produced our highest isobutanol space time yield to date, at 41 g/kg catalyst/h (5 pph Cs, 0.25 pph Cu at 400°C, 1000 psig and 12000 GHSV). Hydrocarbon selectivity was 67%.

Table I compares our targets with 1) our best run to date in terms of isobutanol space time yield and 2) our best run to date in terms of overall performance. We have met or exceeded three of four catalyst development targets. Oxygenate selectivity is our main hurdle.

We replaced stainless steel preheater tubing and fittings with titanium in our reactor system oven in the hope of reducing side reactions. The stainless steel we use contains significant fractions of iron and nickel. Iron and nickel from the stainless steel are believed to catalyze Fischer-Tropsch chemistry. The titanium tubing and fittings we used contain only about 0.09 weight percent iron and no nickel.

We tested a catalyst with 5 pph Cs and 0.18 pph Cu on the Engelhard Zn/Cr support, in both a titanium and a stainless-steel preheater system. Surprisingly, selectivity and space-time yield of hydrocarbons were actually greater with the titanium preheater system than with the stainless-steel preheater system. The space-time yield of total alcohols was very similar for the two systems, but the reactor system with the stainless-steel preheater produced a greater yield of methanol and a lower yield of isobutanol. These results do not support the contention that using a titanium reactor will reduce hydrocarbon formation.

A summary of this work was presented and discussed at the DOE Program Review held at WVU on December 15, 1995.

1.3 Conclusions and Recommendations

The membrane reactor is a promising avenue for HAS. GC/MS can be useful in determining branched-alcohol products obtained over non-sulfided molybdenum catalysts. The Cu/Cs catalysts show promise of meeting all target requirements for HAS. Using a titanium reactor or fittings does not necessarily decrease the production of hydrocarbons during HAS.

1.4 Future Plans

At WVU, work will resume on the detailed kinetics of HAS using the Rotoberty reactor set-up. The use of the membrane reactor will be compared to using a conventional plug-flow reactor. The GC/MS and our in-house library will continue to be used to re-analyze products from previous screening runs using non-sulfide forms of molybdenum catalysts. At UCC, Cu/Cs catalysts will be modified to improve selectivity towards oxygenates.

Table 1. Comparison of Experimental Data with Catalyst Targets

Target Area	Target Value	Highest Isobutanol Space Time Yield*	Best Overall Performance
Catalyst	---	2WMH107A	2WMH102A
Temperature (°C)	---	400	340
1) Oxygenate Space Time Yield	>320 g/kg cat/hr	204	356
2) Selectivity to Oxygenates	>90%	33	35
3) Product Molar Methanol Content	<70%	79	70
4) CO Percent Conversion	>20%	17	30

*41 g isobutanol / kg catalyst / hour

2.1 Introduction

During the past quarter, three runs using (baseline, blend1, and blend2) were conducted.

W have been investigating and quantifying the uncertainty in the projected economics of the alcohol fuels processes. During this quarter, we have defined preliminary uncertainties for input variables, developed the Monte Carlo simulations, and performed some scenario analyses.

During the past quarter, we have made progress in three areas of the optimization algorithm. First, we have obtained preliminary optimization results for the alcohol/gasoline blending facility. Second, we have made progress toward improving the simulated annealing algorithm that we use to do this optimization. Third, we have used the case models that have been developed previously by Task 2 to refine the inputs to the optimization problem.

2.2 Accomplishments, Results, and Discussion

2.2.1 Fuel Testing

During the past quarter, three runs using (baseline, blend1, and blend2) were conducted. Table 2.1 shows the used fuels composition data and the conducted runs settings. Table 2.2 shows the test results for the runs conducted in November and December. Table 2.3 shows a comparison of the baseline and the two blends data.

Figure 2.1 shows plots of the different emissions data in gram per brake horse power hour (gm/bhp-hr) basis versus equivalence ratio. Both blends show a decrease in the CO emissions compared to the baseline. This decrease in CO ranges from ~ 2% for blend1 (3.53%wt. O_2) to ~ 4% for blend2 (3.69% wt. O_2) compared to baseline emissions. Both alcohol blends show a reduction in the THC emissions (~ 10%) compared to that of the baseline. Both blends show a reduced peak of NO_x emissions and reduced CO_2 emissions compared to that of the baseline.

Figure 2.2 shows plots of the exhaust gas temperature, intake mixture temperature, brake engine power, and brake specific fuel consumption versus equivalence ratio for the different tested fuels. Both alcohol blends result in lower intake mixture temperature (~ 4%), higher brake power (~ 2%), and higher brake specific fuel consumption (~ 2% for blend1 and ~ 3.5% for blend2) when compared with baseline data.

2.2.2 Uncertainty, Sensitivity, and Scenario Analyses

The thrust of this work is to identify when an alcohol-fuels plant would be profitable. In terms of inflation and other chronological changes, we have projected the manufacturing costs and the blending values of the alcohol product. As given in the Topical Report, Figure 2.3 shows that the hybrid Shell/Natural-Gas case is initially profitable, but it becomes unprofitable in approximately 2003. (Profitable in this case is defined as meeting the 10% internal rate of return.)

To quantify the uncertainty in the manufacturing cost, we did Monte Carlo simulations using standard uncertainties on the capital and variable costs. For these input cost uncertainties, we used triangular probability distributions. The most probable values were those from the Topical Report. High and Low limits were developed from various sources. For example, the cost for the oxygen plant was varied by ±10%, as this cryogenic technology is very mature. The Shell gasifier, however, was varied by -25% to +35%, based on statements by Shell Corporation.

The results of the manufacturing cost uncertainty study are shown in Figure 2.4. The blending value (based on unleaded regular gasoline, MTBE, and n-butane wholesale prices) shows that there is approximately 10% chance of meeting the benchmark return. The steepness of the cumulative frequency curve is a measure of the certainty of the manufacturing cost. One can use this curve to make decisions on the basis of risk tolerance. We can also investigate the value of uncertainty reduction in the input variables.

From the data generated in the uncertainty analysis simulations, we performed sensitivity analyses to determine which uncertain inputs had the greatest effect on the manufacturing cost. The Shell gasifier capital cost, the electrical power credit, and the coal cost were significantly more important on this basis than were the other costs. Therefore, we have developed the scenario analyses for the process depicted in Figures 2.5 and 2.6. The "+" symbol on these two graphs denotes the regions where the benchmark return is satisfied. Thus, one can determine the required power credit or maximum coal cost required to attain profitability if the gasifier can be acquired for a discount. These scenario analyses define the profitability frontier that must be crossed before the alcohol fuels process is viable.

2.2.3 Simulated Annealing Optimization

For the alcohol fuel blending facility, we have used preliminary data to obtain some results for the optimization problem. These results are not exact because not all the necessary input data were available, and reasonable estimates had to be made in place of these data. Nevertheless, the results are useful in that they give us a qualitative description that can be improved later with more complete data. The data that were collected were for an alcohol facility producing 5.1 billion liters per year of mixed alcohols to be blended with varying flow rates of a gasoline pool. The results obtained are shown graphically in Figure 2.7.

In the direction of increasing gasoline flow, we notice an initial drop in the profitability, followed by increasing profitability until it levels off and remains constant. Note that all the profits for this study were negative. This is expected because the blending value of the alcohol product is currently less that the manufacturing cost. (See Case 5 in the Topical Report.) The initial drop off is because we would not be using all of the alcohol we produce. Between a gasoline flow rate of 600,000 and 700,000 liters per hour, we begin to use all the alcohol we produce. At these flow rates, the gasolines produced would have higher octane numbers and/or lower Reid vapor pressures than are required. This explains why the profitability continues to increase as the gasoline pool expands. Finally, there is a gasoline pool size at which all the octane numbers and Reid vapor pressures are at their constraints. At this point, there would be no further change in profitability with respect to increasing gasoline pool size.

The most important data that were estimated for this study were the outlet alcohol concentrations from the reactor. Information in this area will need to be obtained from Task 1 before better results can be provided for the optimization. Also, we are still modifying the cost equations used in the program as well as some of the flow patterns in the distillation section of the process. However, in these areas, we have or can obtain whatever information we require.

The second area we have made progress in concerns the simulated annealing algorithm that we use to obtain results from the blending facility optimization. We have been and continue to run experiments on other chemical engineering problems in order to learn how to operate the algorithm more efficiently. These improvements will be implemented at the same time that other modifications to the program are made for future optimization work.

The third area we have worked on involves using the case models to refine the inputs to the blending problem. Specifically, we can calculate the effective cost of synthesis gas at varying hydrogen to carbon monoxide ratios and total flow rates. For any particular case model, we can remove all parts of the process that occur after the synthesis gas is made and cleaned. This allows us to calculate a cost for it without knowing the particulars about the effect of hydrogen to carbon monoxide ratio on reaction products. These cost data are being regressed into equations that will be put directly into the optimization program. This results not only in better accuracy but will reduce future computation time by removing the need to make all the calculations required in the gasification process of the facility during optimization. Any parts of the problem removed from the case models are then, necessarily, inserted into the optimization program.

2.3 Conclusions

In fuel testing, emissions from different alcohol blends have been measured and both blends show a decrease in the CO emissions compared to the baseline. Additionally, both alcohol blends show a reduction in the THC emissions (~ 10%) compared to that of the baseline. Finally, both blends show a reduced peak of NO_x emissions and reduced CO_2 emissions compared to that of the baseline.

A Monte Carlo uncertainty study on the manufacturing shows that there is approximately 10% chance of meeting the benchmark return. The Shell gasifier capital cost, the electrical power credit, and the coal cost had the greatest effect on the manufacturing than the other costs.

For the alcohol fuel blending facility, optimization shows that in the direction of increasing gasoline flow, we notice an initial drop in the profitability, followed by increasing profitability until it levels off and remains constant. This is expected because the blending value of the alcohol product is currently less that the manufacturing cost.

2.4 Future Work

For the two runs conducted with alcohol blends, unburned alcohol samples in the exhaust gas (dissolved in distilled water using bubbler) are sent to the gas chromatography lab to be analyzed. DNPH (2,4-dinitrophenylhydrazine-coated silica) cartridges used to trap aldehydes are sent for analysis. As soon as these results become available they will be reported.

We shall continue to develop our uncertainty, sensitivity, and scenario analyses to get a better understanding of the nominal results presented in the Topical Report. We shall develop, test, and implement our simulated annealing optimization strategies on the downstream reaction/separation trains of the process. In all of these analyses, we will incorporate the catalyst and reactor-design results of Task I when they become available.

Table 2.1: Test Settings Specific Data

Fuel Composition (Volume Fractions)

	Baseline	Blend 1	Blend 2
Indolene:	1	0.9	0.9
Methanol:	0	0	0.01
Ethanol:	0	0.085	0.075
Propanol:	0	0.012	0.012
Butanol:	0	0.002	0.002
Pentanol:	0	0.001	0.001

Fuel Molecular Structure

	Baseline	Blend 1	Blend 2
Carbon:	8	7.419	7.409
Hydrogen:	15	14.138	14.118
Oxygen:	0	0.1	0.1
Nitrogen:	0	0	0
% wt. Oxygen:	0	3.53	3.69
Stoichiometric A/F:	14.51	13.95	13.92
Fuel Density (kg/m3):	742	748	748

Engine Settings

Spark Timing (deg btdc): 25
Compression Ratio: 7:1

In Line Hydrocarbon Analyzer Settings

Span Gas: 1500 ppm propane
Range: 100
Fuel Regulator Pressure: 25 (psig)
Air Pressure Regulator: 15 (psig)
Sample Pressure Regulator: 3 (psig)
Oven Temperature: 235 (F)
Sample Line Temperature: 240 (F)

Dilution Cart Settings

Sample Line Temperature: 240 (F)
Dilution Ratio: 7.69
Mass Flow Controllers Calibration Date: 11/10/95

Quality Control

Check on Dilution Ratio

Test Date:	11/21	11/22	11/24
Span Gas Conc.:	4500	4500	4500
Diluted Span Gas Conc.:	584	583	581
Calc. Span Gas Conc.:	4444	4436.4	4421
Relative Error (%):	1.242	1.4124	1.754

In Line Hydrocarbon Analyzer Response Factors

Methanol:

Cylinder Conc. (ppmC):	106
FID Reading (ppmC):	62
Response Factor:	0.585

Ethanol

Cylinder Conc. (ppmC):	189.8
FID Reading (ppmC):	120
Response Factor:	0.632

Table 2.2: Test Result Data

Num.	Fuel Type	Sample ID.	Engine			Equiv. ratio	Tmprtr		Exhaust Gas Emissions (gram/bhp-hr)				Fuel
			Speed (rpm)	Torque (ft-lbf)	Power (hp)		Exhaust (f)	Intake (f)	CO	CO2	Nox	HC	BSFC gm/bhp-hr
1	Indolene	1121B10.BSE	900	14.05	2.41	0.74	1002	119.8	3.97	983.98	23.36	3.05	293.07
2	Indolene	1121B00.BSE	902	15.25	2.62	0.80	1031	118.9	2.98	927.84	27.05	3.15	288.66
3	Indolene	1121B01.BSE	901	15.97	2.74	0.85	1063	118	2.60	982.12	24.55	3.18	294.34
4	Indolene	1121B02.BSE	899	16.22	2.78	0.86	1070	117.5	2.68	969.65	23.14	3.29	293.05
5	Indolene	1121B03.BSE	901	16.37	2.81	0.87	1078	117.3	4.96	962.95	21.06	3.53	292.28
6	Indolene	1121B04.BSE	900	16.7	2.86	0.94	1060	116.1	74.65	908.81	12.20	5.36	309.47
7	Indolene	1121B05.BSE	899	16.62	2.84	1.01	1031	115.1	155.79	832.66	6.60	6.29	334.08
8	Indolene	1121B06.BSE	899	16.47	2.82	1.07	1000	113.7	242.86	757.65	3.53	6.83	355.00
9	Indolene	1121B07.BSE	900	16.3	2.79	1.14	967	112.4	350.77	702.67	1.89	8.27	385.37
10	Indolene	1121B08.BSE	900	16.18	2.77	1.24	935	111	462.64	649.96	1.10	9.71	419.39
11	Indolene	1121B09.BSE	899	16.15	2.76	1.29	912	109.9	536.07	596.62	0.76	10.96	438.87
12	Indolene	1129B11.BSE	900	13.58	2.33	0.71	989	119.4	2.73	1002.99	22.45	2.84	295.48
13	Indolene	1129B10.BSE	901	15.13	2.60	0.79	1024	118.2	2.23	970.97	32.98	2.69	292.65
14	Indolene	1129B08.BSE	901	16.19	2.78	0.86	1062	117.1	2.65	977.53	23.84	2.51	292.94
15	Indolene	1129B05.BSE	902	16.73	2.87	1.01	1030	113.9	161.25	831.20	5.78	5.51	332.03
16	Indolene	1129B01.BSE	899	16.62	2.84	1.12	984	111.9	306.95	745.93	2.16	6.94	372.04
17	Indolene	1129B04.BSE	899	16.48	2.82	1.22	945	110.4	432.76	660.68	1.04	8.41	409.66
18	Blend 1	1122B00.BL1	902	12.79	2.20	0.67	971	117.4				2.23	309.76
19	Blend 1	1122B01.BL1	903	14.69	2.53	0.75	999	115.9	2.27	920.47		2.64	297.90
20	Blend 1	1122B02.BL1	898	16.37	2.80	0.83	1053	113.5	3.27	898.79	24.02	2.67	294.54
21	Blend1	1122B03.BL1	901	17.11	2.94	0.90	1077	111.9	22.83	901.05	15.23	3.84	302.94
22	Blend1	1122B04.BL1	900	17.11	2.93	0.97	1049	110.2	95.54	865.62	8.99	4.72	326.61
23	Blend1	1122B05.BL1	899	16.94	2.90	1.02	1026	109.8	129.51	844.06	7.50	5.31	343.91
24	Blend1	1122B10.BL1	902	16.74	2.87	1.07	992	107.9	268.27	769.17	3.23	6.07	366.90
25	Blend1	1122B11.BL1	903	16.8	2.89	1.14	972	106.5	331.80	726.12	1.96	7.45	390.11
26	Blend1	1122B08.BL1	898	16.52	2.82	1.24	932	104.9	457.98	659.20	1.24	8.59	432.07
27	Blend1	1129B00.BL1	899	12.61	2.16	0.67	974	118.7	3.27	1022.88	9.47	2.87	315.23
28	Blend1	1129B09.BL1	901	15.18	2.60	0.79	1019	115.6				2.48	304.13
28	Blend1	1129B11.BL1	899	16.9	2.89	0.88	1077	113.4	4.57	953.60	23.28	2.97	299.92
29	Blend1	1129B10.BL1	901	16.99	2.91	1.02	1030	110.3	139.96	764.13	5.33	5.05	344.61
30	Blend1	1129B08.BL1	900	16.74	2.87	1.14	975	107	288.30	665.32	1.68	6.71	391.56
31	Blend1	1129B05.BL1	902	16.57	2.85	1.30	928	104.5	406.14	556.13	0.56	8.71	452.89
32	Blend2	1124B01.BL2	896	12.93	2.21	0.67	969	117.3	4.48	1010.22	11.17	2.71	311.72
33	Blend2	1124B11.BL2	902	14.58	2.50	0.75	996	116.2	2.47	956.99	25.96	2.45	303.36
34	Blend2	1124B10.BL2	901	16.34	2.80	0.84	1057	113.2	2.39	962.18	23.55	2.58	300.52
35	Blend2	1124B08.BL2	899	17.07	2.92	0.99	1046	110.2	111.58	861.04	7.83	4.79	335.13
36	Blend2	1124B04.BL2	902	16.69	2.87	1.17	970	106.8	338.60	693.95	1.33	7.08	404.42
37	Blend2	1124B05.BL2	899	16.63	2.85	1.22	938	104.8	438.57	625.24	0.60	8.28	427.47
38	Blend2	1130B11.BL2	901	13.6	2.33	0.73	982	117	2.72	984.30	23.62	2.43	314.78
39	Blend2	1130B10.BL2	901	15.27	2.62	0.80	1023	114.5	2.33	946.94	30.42	2.48	305.09
40	Blend2	1130B08.BL2	900	16.84	2.89	0.92	1073	111.6	25.98	882.34	15.33	3.89	311.88
41	Blend2	1130B00.BL2	901	16.77	2.88	1.00	1034	109.9	130.12	778.93	6.59	5.04	341.62
42	Blend2	1130B05.BL2	901	16.59	2.85	1.10	986	107.4	268.65	689.30	2.46	6.44	378.21
43	Blend2	1130B01.BL2	901	16.42	2.82	1.22	935	105	450.79	614.93	1.05	8.44	426.86

Table 2.3: Comparison of Baseline & Blends Data

Equivalence Ratio Range		BASELIN	Difference (percent)	
			BLEND1	BLEND2
min	max	Intake mixture temperature (f)		
0.75	0.95	117.65	-3.41	-3.61
0.95	1.05	114.77	-4.16	-4.45
1.05	1.25	111.97	-4.76	-4.69
min	max	Exhaust gas temperature (f)		
0.75	0.95	1050.90	-0.39	-0.91
0.95	1.05	1037.95	0.31	0.55
1.05	1.25	968.37	-0.33	-0.13
min	max	Brake power (hp)		
0.75	0.95	2.72	2.32	0.65
0.95	1.05	2.86	2.46	1.85
1.05	1.25	2.81	1.63	1.04
min	max	Carbon monoxide [CO] (gm/bhp-hr)		
0.75	0.95	16.13	-17.03	7.74
0.95	1.05	144.23	-15.37	-13.89
1.05	1.25	350.40	-4.25	-3.84
min	max	Carbon dioxide [CO2] (gm/bhp-hr)		
0.75	0.95	955.20	-5.32	-3.03
0.95	1.05	848.96	-1.83	-4.25
1.05	1.25	707.90	-1.39	-4.78
min	max	Nitric oxide [NOx] (gm/bhp-hr)		
0.75	0.95	23.10	-6.61	-3.73
0.95	1.05	7.49	3.30	-5.60
1.05	1.25	1.89	8.51	-15.06
min	max	Hydrocarbons [THC] (gm/bhp-hr)		
0.75	0.95	3.44	-10.40	-10.87
0.95	1.05	5.76	-14.41	-13.78
1.05	1.25	7.91	-8.44	-9.39
min	max	BSFC (gm/bhp-hr)		
0.75	0.95	295.65	2.31	4.27
0.95	1.05	329.05	2.17	2.98
1.05	1.25	385.70	2.71	3.56

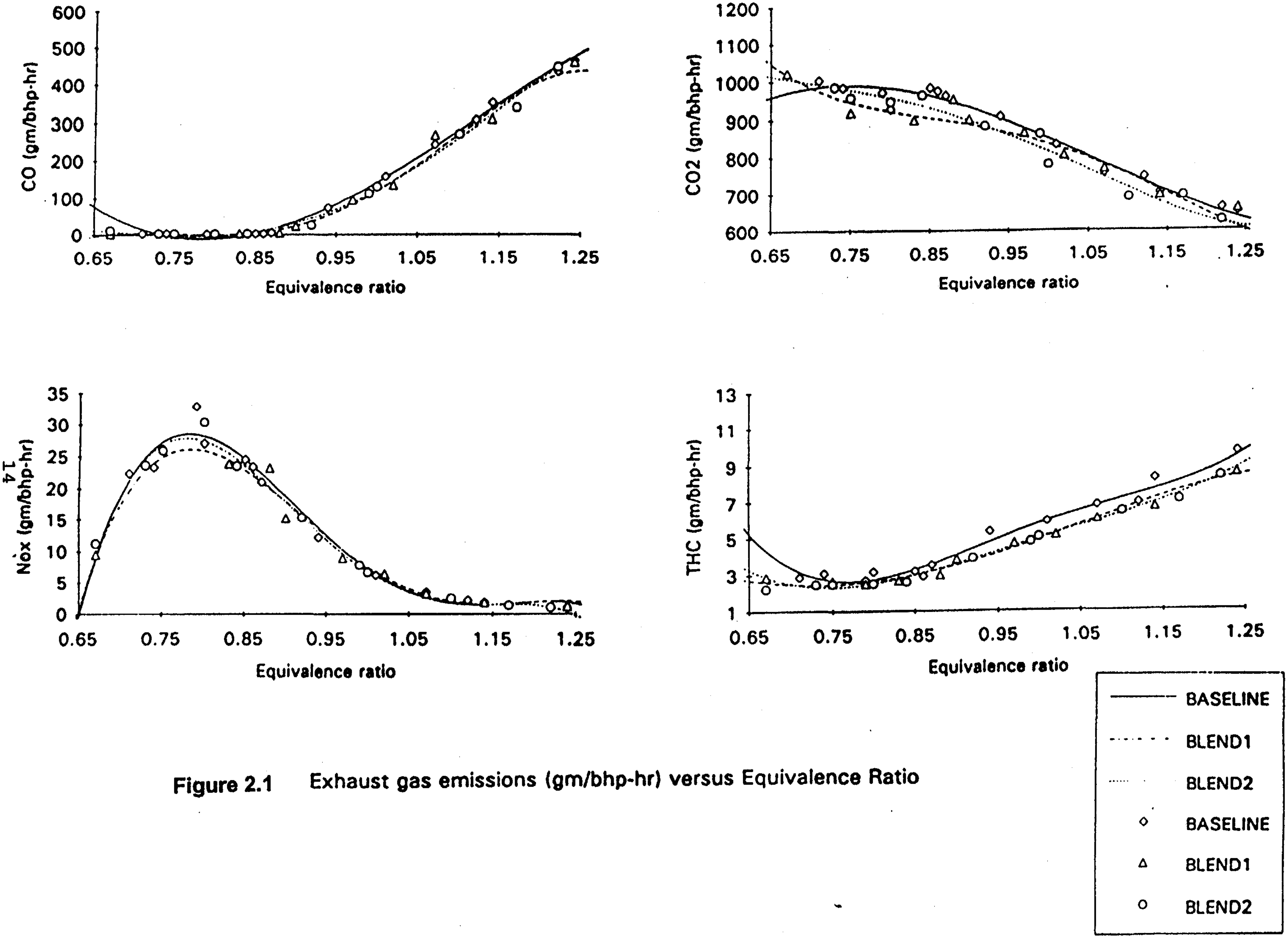

Figure 2.1 Exhaust gas emissions (gm/bhp-hr) versus Equivalence Ratio

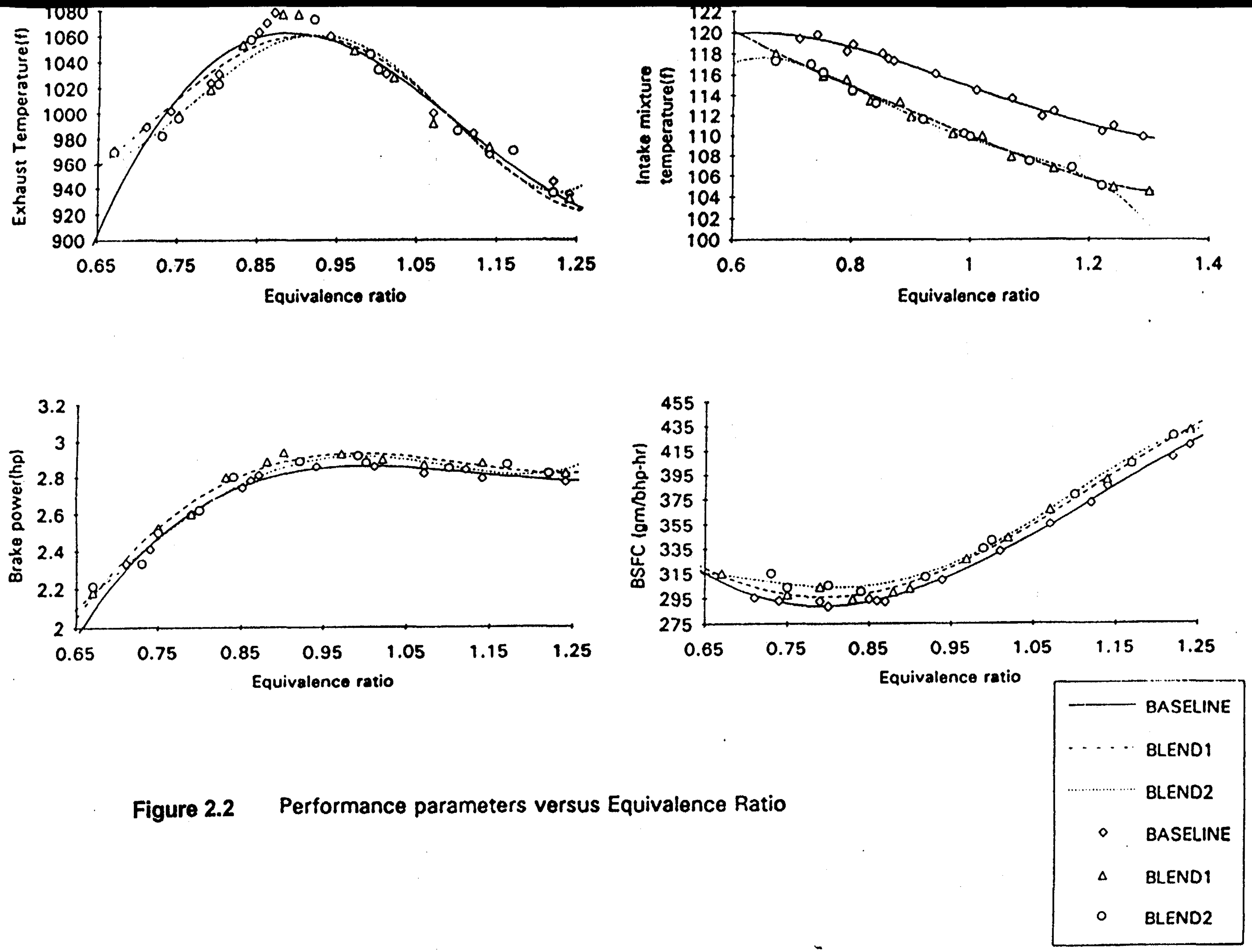

Figure 2.2 Performance parameters versus Equivalence Ratio

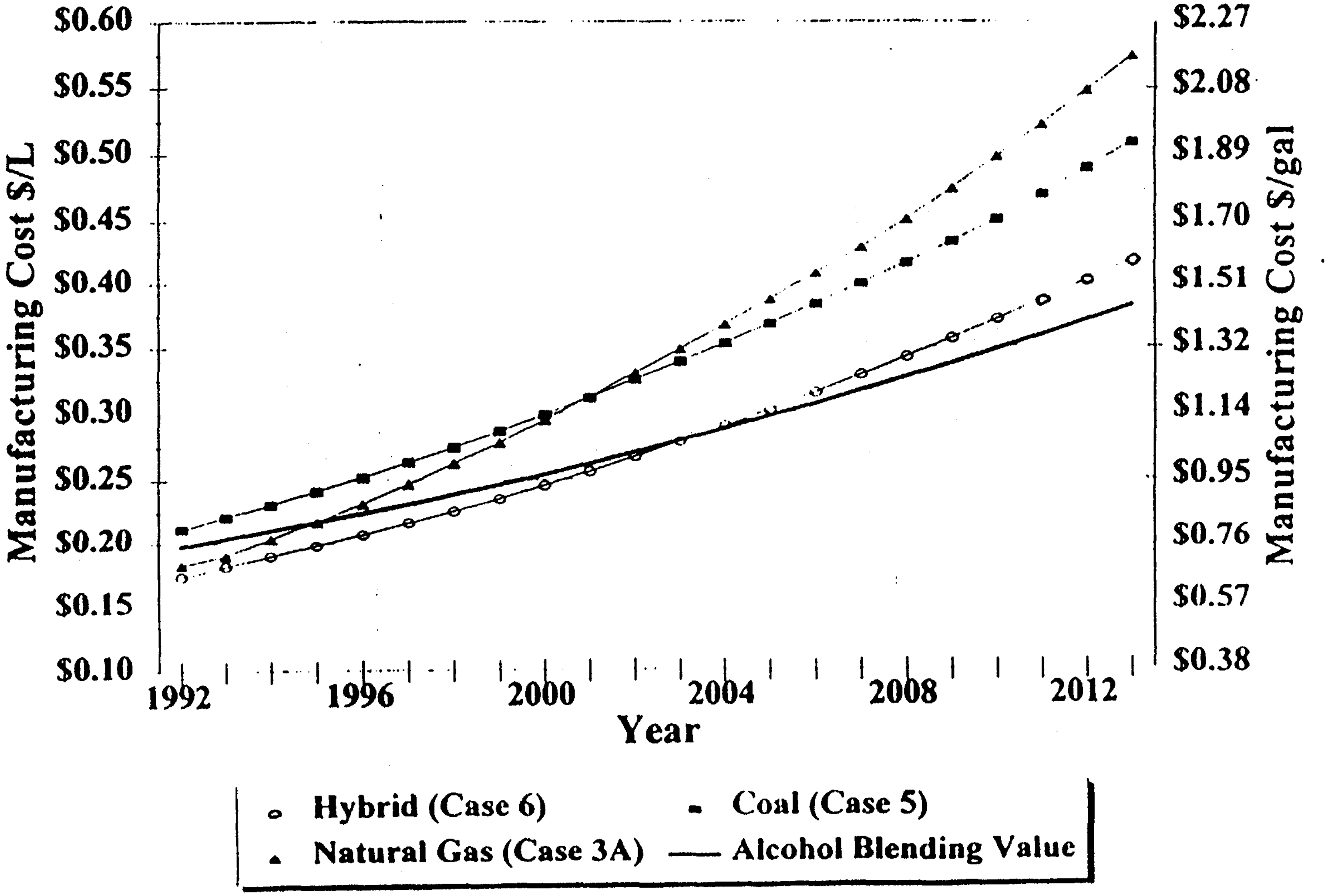

Figure 2.3. Projected Manufacturing Costs and Blending Values

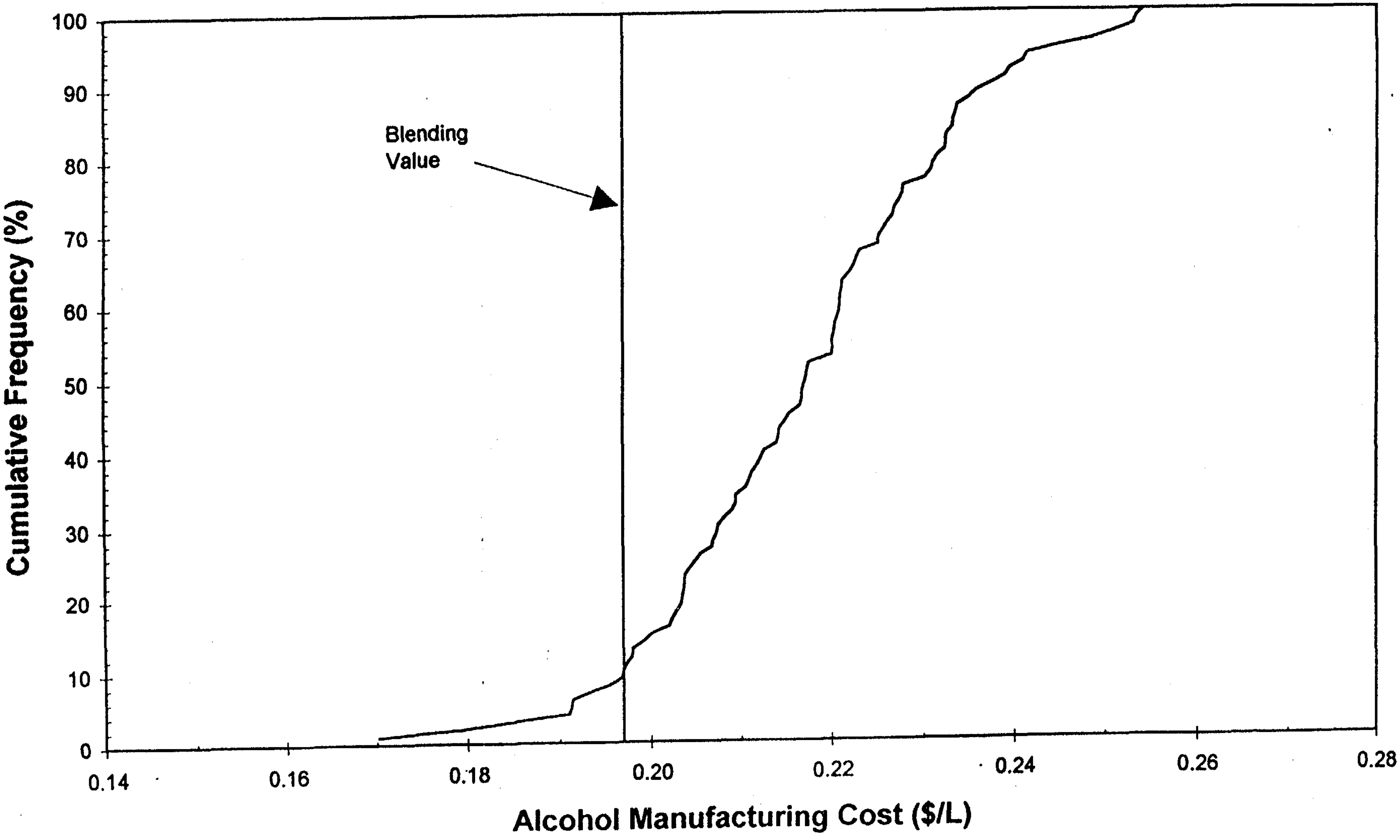

Figure 2.4. Manufacturing Cost Uncertainty (Shell, full-scale)

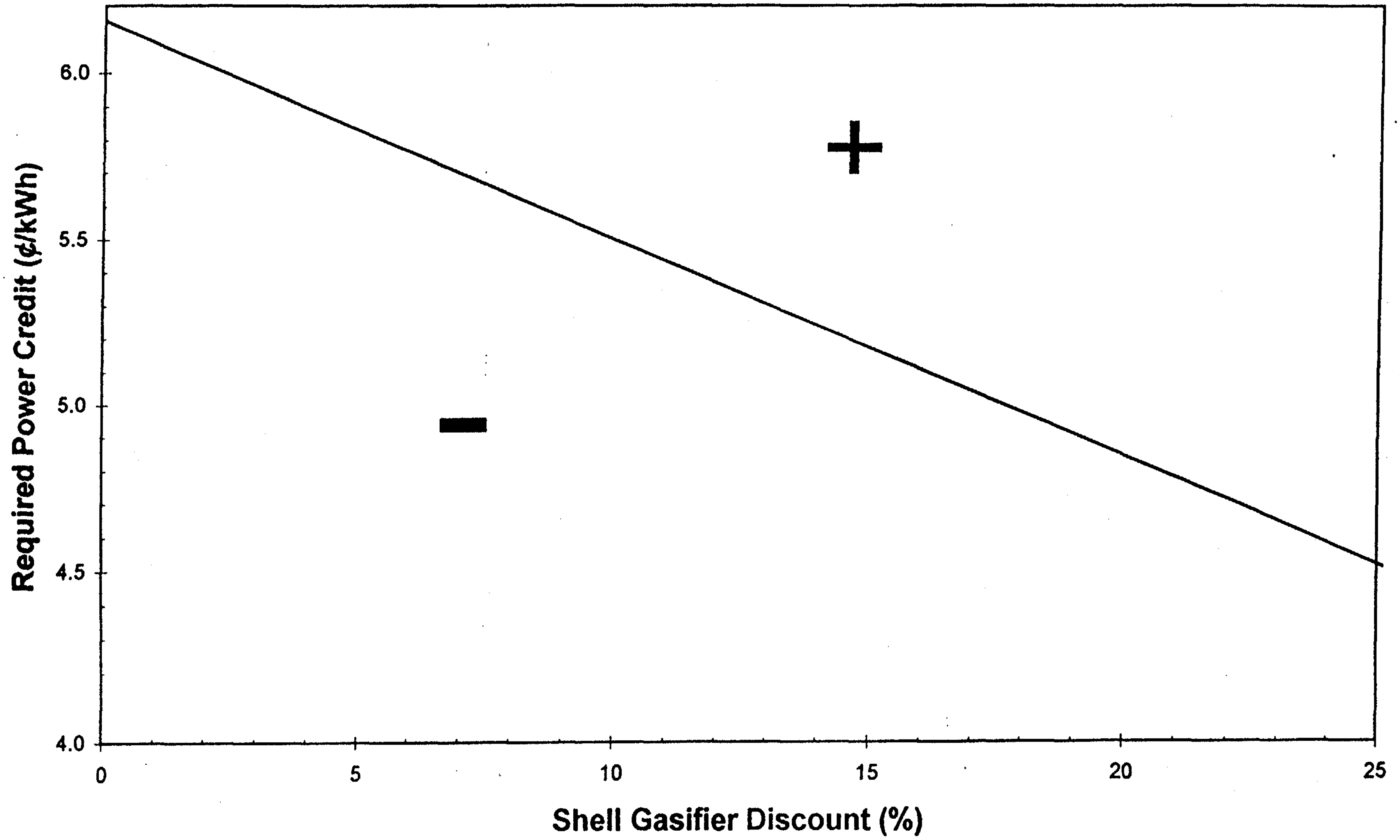

Figure 2.5. Scenarios for Benchmark Return (Shell, full-scale)

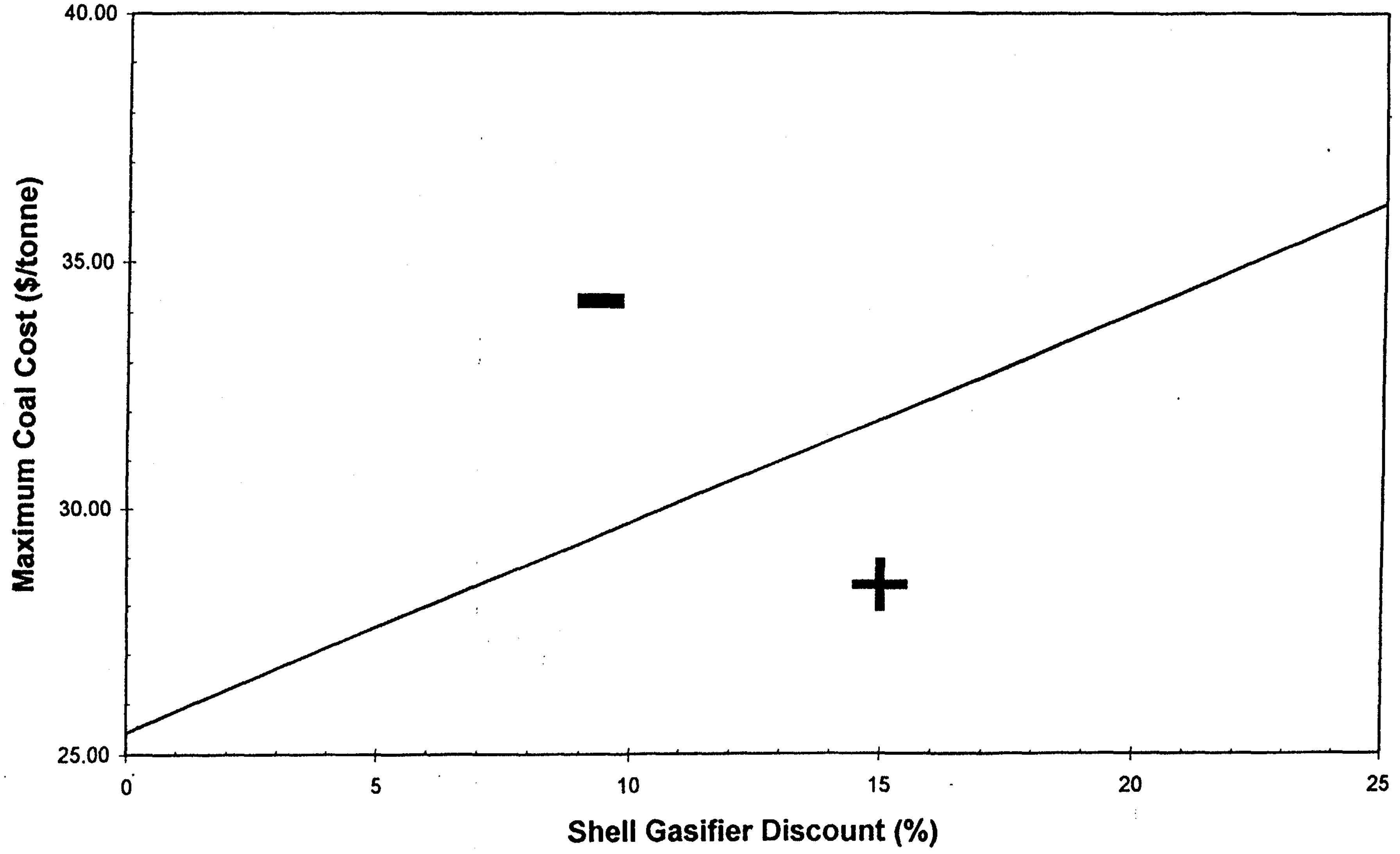

Figure 2.6. Maximum Coal Cost for Benchmark Return (Shell, full-scale)

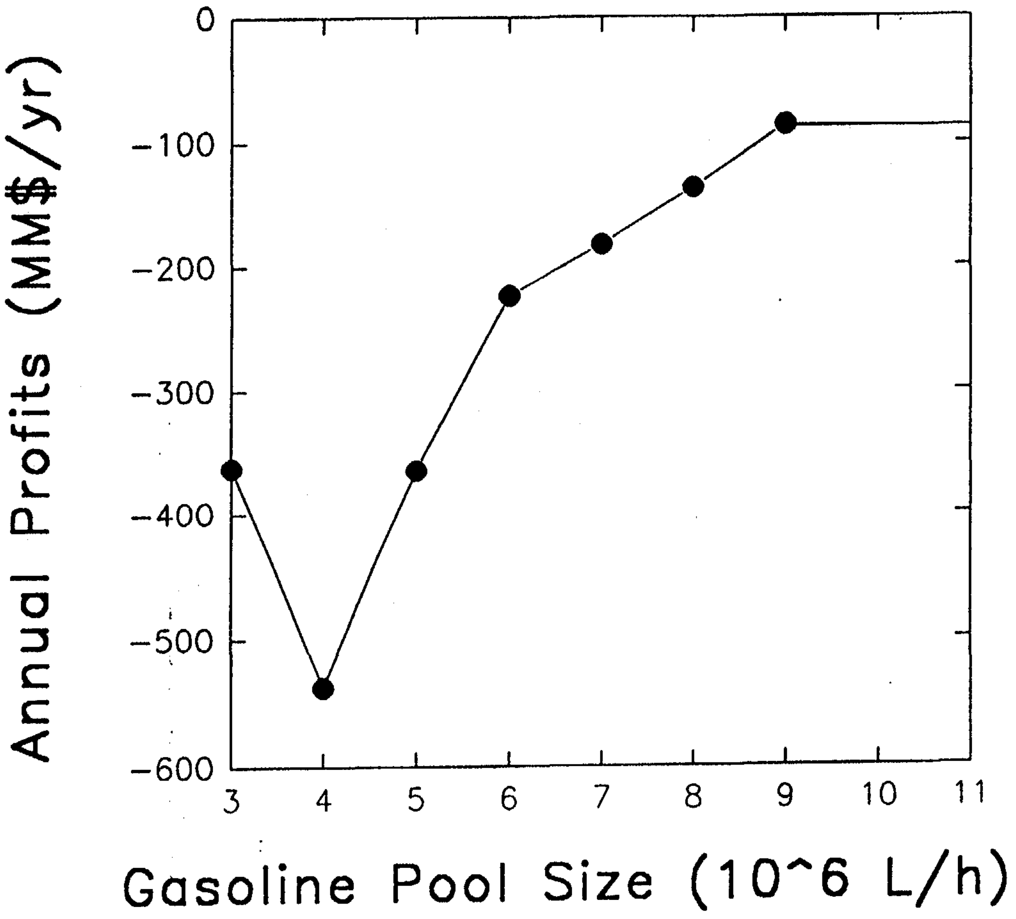

Figure 2.7. Preliminary Optimization Results for Facility