6. Results and Discussion

6.1 Economics of Designs

Table 6.1 is a summary of capital costs for the seven cases at all scales. Individual unit costs are tabulated in Appendix H.

Table 6.1 Capital Costs for Cases (in millions of dollars)				
Case #	x1	x2	x4	x8
1	562.80	958.96	1,778.88	3,311.88
2	1,817.14	3,438.22	--	--
3	335.89	562.28	981.88	1,748.10
4	650.27	1,182.33	2,171.06	4,076.87
5	629.92	1,138.72	2,066.51	3,926.76
6	416.61	734.38	1,347.78	2,488.20
7	999.63	--	--	--

Figure 6.1 shows the manufacturing cost of higher alcohols for Cases 1-6 at different scales. The lowest scale (x1) produces 636 million liters/yr (4 MM bbl/yr). It is apparent that the most attractive option is to produce higher alcohols from synthesis gas produced by the steam reformation of natural gas available at Gulf Coast prices. The main reason for this result is the low capital investment associated with the natural gas reformation process. From Table 6.1, it can be seen that this investment is significantly lower than that for the other cases considered for the same alcohol output. Of the cases using coal as a raw material, the Shell Gasifier with natural gas is the best case, and can be better than natural gas, as long as the natural gas price is above $2.45/MM BTU. The best coal case also involves a Shell Gasifier, and can be better than Shell coal/natural gas hybrid case, if the natural gas price exceeds $4.94/MM BTU. Furthermore, the economic advantages of a Shell or Texaco gasifier over a Lurgi gasifier are clear. The manufacturing costs in Figure 6.1 represent a 10% real rate of return on capital over a 20 year plant life without considering the effects of taxes. If a plant life of 10 years is used, which is more typical in the chemical process industry, then all of the curves in Figure 6.1 using coal gasification will shift upwards, making natural gas the clearly superior option. The effects of differential inflation rates on coal and natural gas are discussed later in this section.

On Figure 6.1, the curves labeled Case 3A and Case 3B reflect the sensitivity of manufacturing costs to changes in natural gas prices. In Case 3A, the cost of natural gas used is $106/1000 std m^3, which is a typical industrial price in West Virginia. In Case 3B, the cost is a typical Gulf Coast price of $61.8/1000 std m^3. In both cases, excess hydrogen is assigned a credit of approximately one-third that of natural gas, based on the respective heating values. These cases are detailed in Appendix C.

Figure 6.1

Manufacturing Cost Comparison
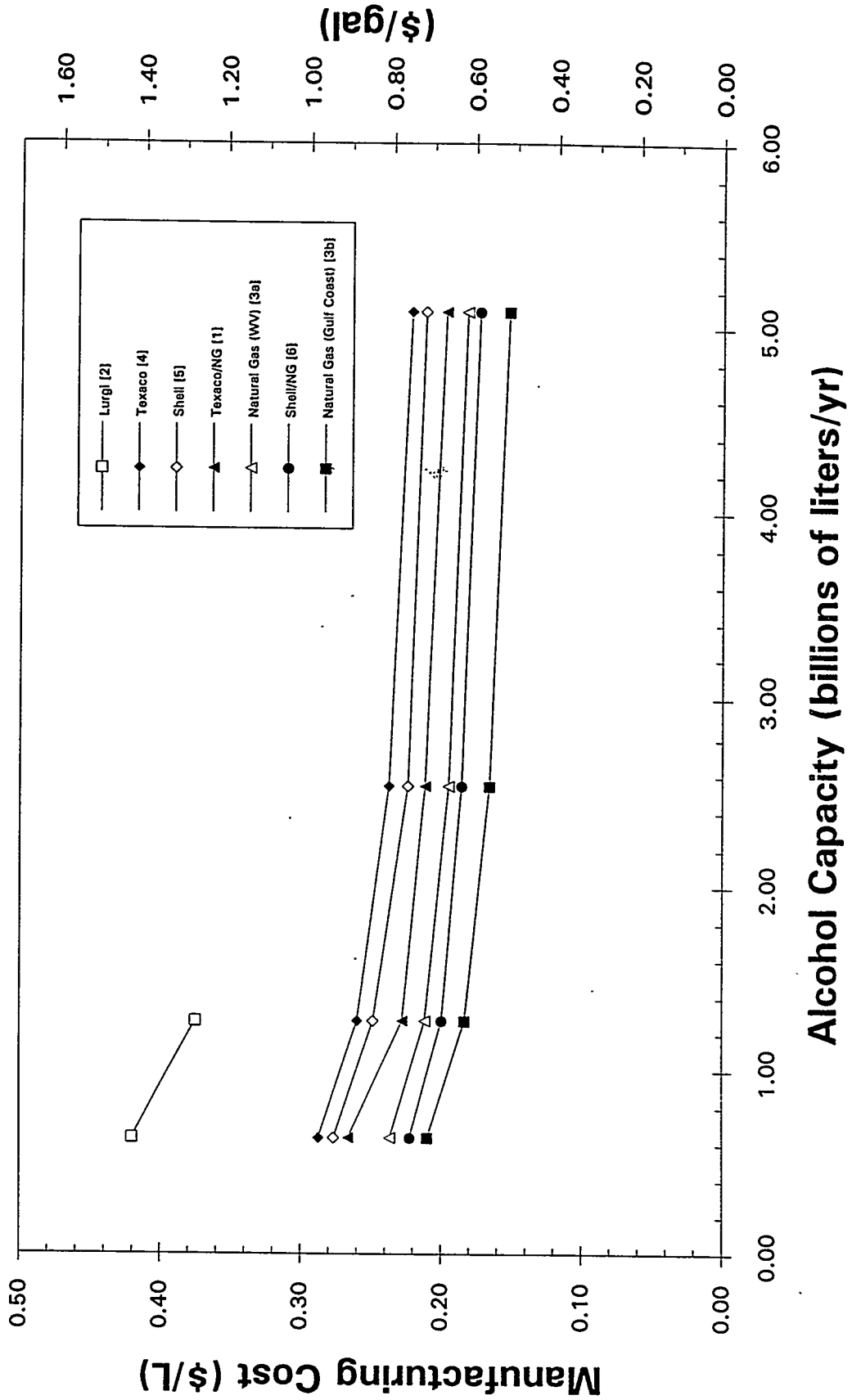
Considering the cases that use coal as a raw material, the process based around the Lurgi Gasifier (Case 2) is by far the worst option and is not considered further in this discussion. Of the remaining cases, all of which use modern oxygen-blown gasifiers, the cases which utilize a mixed feed of coal and natural gas (Cases 1 and 6) are superior, in terms of unit cost of product, to their respective counterparts (Cases 4 and 5) which use coal as the only feed material. Again the main reason for this result is the reduced capital investment associated with the cases using natural gas which in turn is mainly due to the reduced cost of the gasifier and oxygen plant. Comparisons between the Texaco and Shell Gasifiers, with or without a natural gas feed, (Case 1 vs. 6 and Case 4 vs. 5), show the Shell to be slightly superior to the Texaco. For the hybrid cases (1 and 6), the substantial difference in manufacturing costs results from the increased natural gas requirement for Case 6 (Shell). This case, therefore, benefits from the fact that natural gas is a less expensive source of hydrogen than is syngas shifting.

In all of the cases, light hydrocarbon gases are separated from the alcohol fuel product, with a fraction recycled to the reactor and the remainder used to produce power in combustion turbines. The methane in the recycle was held constant at 21%, as in previous designs [7]. Optimization of the fraction recycled for each case does not appreciably alter the results in Figure 6.1, except for the Lurgi gasifier. For this case, the manufacturing cost is reduced by about $0.35/gal at the optimum recycle fraction. The Lurgi gasifier is still the worst case, but not by as large a margin as in Figure 6.1.

From Figure 6.1, it is clear that natural gas is superior to coal as a source of alcohol fuels, as long as the price of natural gas is less than $2.45/MM BTU (based on Case 6). However, it has been reported that natural gas suppliers are reluctant to provide long term contracts at this price, even with built-in inflation clauses [19]. The manufacturing cost of the alcohol derived from natural gas is a strong function of the raw material cost. The two cases, 3A and 3B, represent reasonable bounds for the cost of natural gas and clearly illustrate the sensitivity to raw material costs. Additional savings could be achieved in both cases 3A and 3B if the pressure-swing adsorption unit were replaced with a separation process that delivered the hydrogen-stripped syngas at close to the pressure of the feed to that process, e.g., membrane separation.

The cost of producing syngas from coal or from coal and natural gas is currently greater than producing it from natural gas only. This is primarily a result of the high capital investment for the gasifier and accompanying cryogenic oxygen plant. This higher investment outweighs the benefit of using a cheaper raw material, coal. The only way for coal based processes to be more competitive than natural gas under all conditions is either for the relative price of coal and natural gas to change or for a major development to occur in coal gasification technology. The effects of both are illustrated in Figures 6.2 and 6.3. Price variations would have greater impact on the natural gas reference cases, since raw material costs for these cases are a larger portion of the total annualized cost. Therefore, the competitiveness of the coal-based cases would be enhanced more by increases in the price of natural gas than by decreases in coal cost.

Figure 6.2

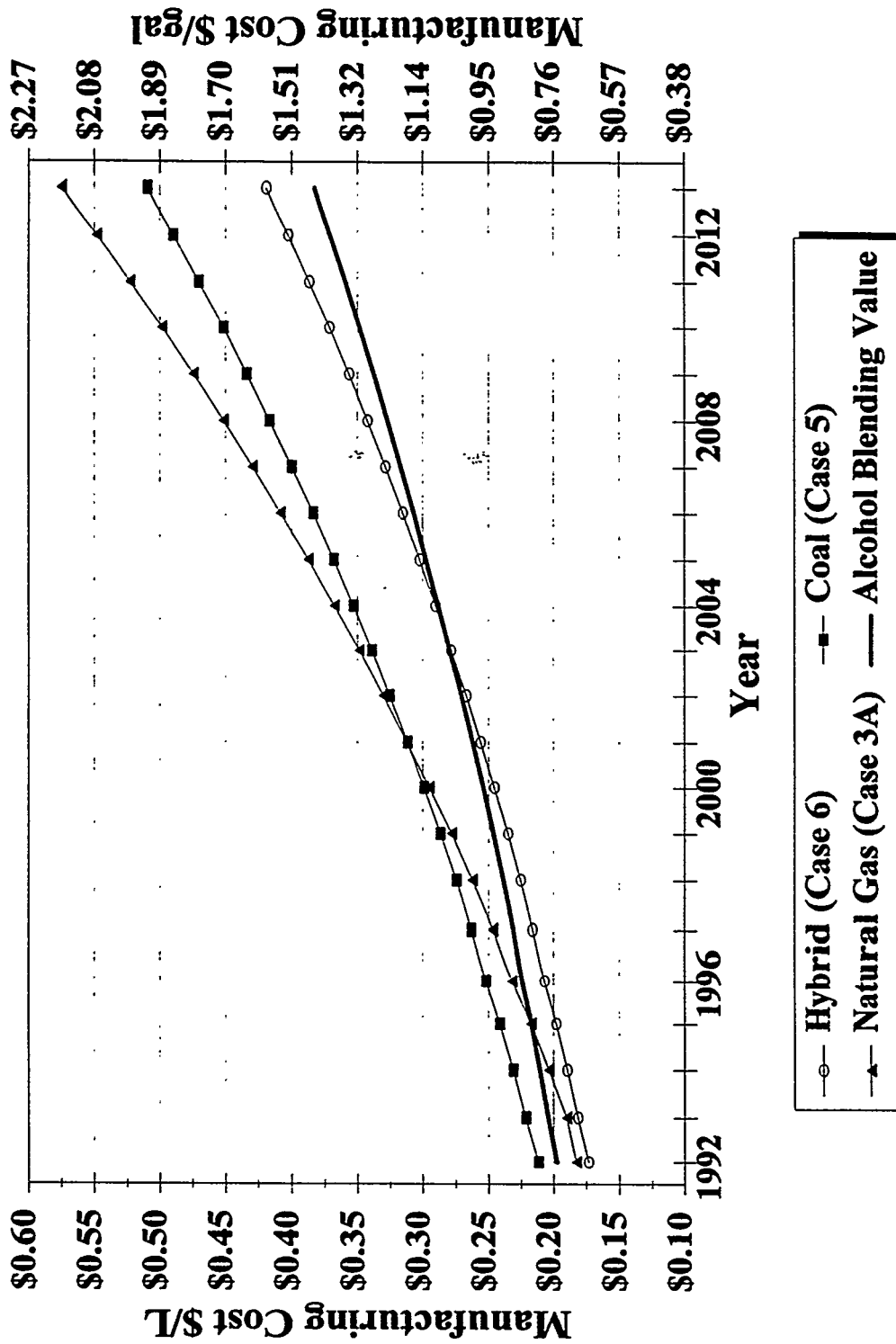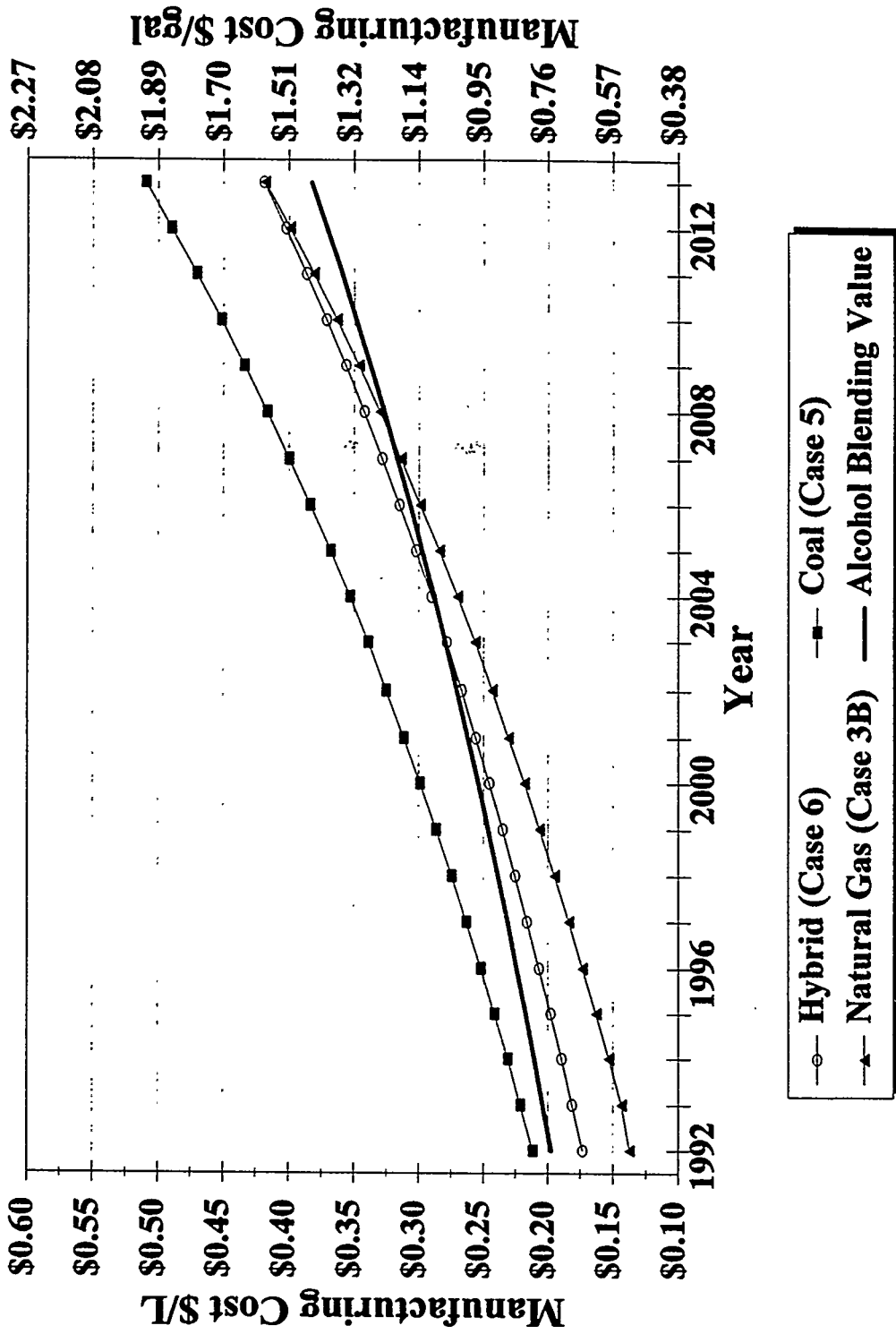Projected Manufacturing Costs
and Blending Values

Figure 6.3

**Projected Manufacturing Costs
and Blending Values**

⊸ Hybrid (Case 6)	⊸ Coal (Case 5)
⊸ Natural Gas (Case 3B)	— Alcohol Blending Value

The relative profitability of higher alcohol fuel additives with respect to MTBE depends upon both the initial manufacturing costs and the rate of change of these costs with time. Figures 6.2 and 6.3 show the results of an analysis of the relative costs of higher alcohol fuel additives assuming the following initial costs: coal, $33/metric ton; oil, $0.116/liter ($18.45/bbl); MTBE, $0.223/liter ($35.49/bbl). The difference between Figures 6.2 and 6.3 is the different starting price of natural gas in Case 3. The starting price of natural gas in Case 6 is the West Virginia price, since the desired comparison is between a West Virginia hybrid plant and either a West Virginia or a Gulf Coast natural gas only process. Table 6.2 shows the assumed inflation rate for each component of the economic analysis.

Table 6.2 Assumed Inflation Rates	
coal [20]	1.7%
natural gas [20]	3.5%
equipment and labor [21]	3.9%
hydrogen [20]	3.5%
slag [21]	3.2%
electricity [20]	0.55%
sulfur (estimated)	0.09%
alcohol fuel product*	3.2%
*assumed to be the same as the inflation rate of crude oil [20]	

As can be seen in Figures 6.2 and 6.3, the cheapest source of higher alcohol fuel additives depends upon the assumed starting price for natural gas. Different relative cost increases will change the ranking over time. From Figure 6.2 (natural gas at $106/1000 m³), it appears that the hybrid case may be the most profitable relative to the alcohol blending value until 2003. After 2003, it appears that none of these cases will be profitable. From Figure 6.3 (natural gas at $61.8/1000 m³), the hybrid case the natural gas case appears to be the most profitable until 2008. However, we have estimated the marginal producer's cost of MTBE as $0.159/liter ($0.600/gal). If the price of MTBE declines, so would the relative values of the other blending agents. Therefore, if the alcohol fuel product must compete with MTBE at the marginal producer's cost of MTBE, then none of the cases (neither coal, natural gas, nor a hybrid) would be profitable.

6.2 Energy Efficiency of Designs

Using the Energy Park concept, it is suggested that overall energy efficiencies may be used as a screening mechanism. Therefore, the overall thermal efficiencies and distribution of energy flows for the various cases are calculated to assess the viability of the various processes. These calculations are based upon the original design capacities of approximately 1.9 million liters of mixed alcohol/day (12,000 bbl/day). The total energy inputs and outputs for these cases are summarized in Table 6.3 and illustrated graphically in Figures 6.4 and 6.5. The most efficient processes are those which involve the use of
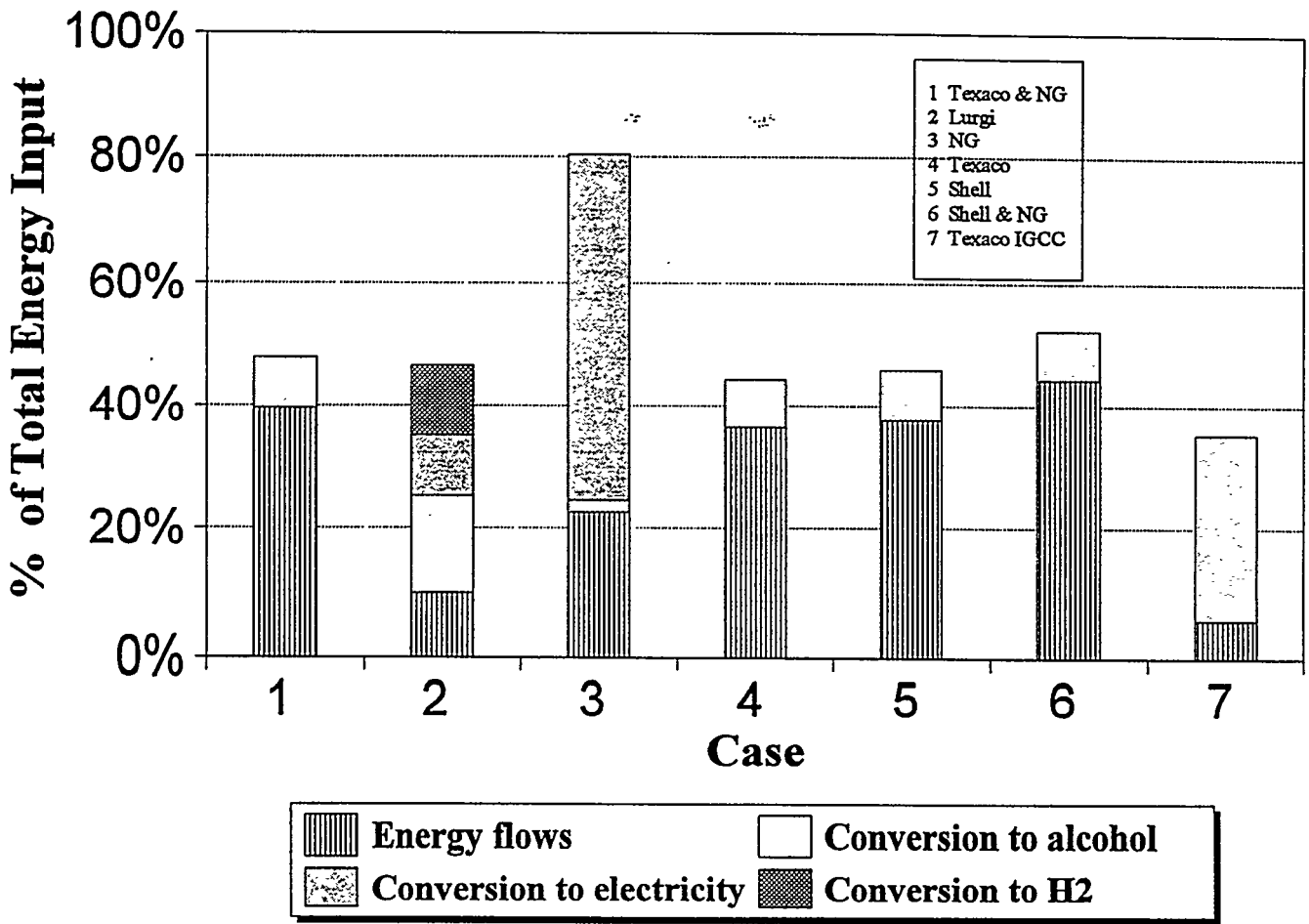
Figure 6.4
Overall Efficiency & Distributions

Legend:
- **Energy flows**
- **Conversion to electricity**
- **Conversion to alcohol**
- **Conversion to H2**

Case key:
1 Texaco & NG
2 Lurgi
3 NG
4 Texaco
5 Shell
6 Shell & NG
7 Texaco IGCC

Figure 6.5
Energy Production and Consumption

Legend:
- 1 Texaco & NG
- 2 Lurgi
- 3 NG
- 4 Texaco
- 5 Shell
- 6 Shell & NG
- 7 Texaco IGCC

Y-axis: GJ/Hr (Thousands)
X-axis: Case

Legend:
- Energy flows
- Conversion to H2
- Conversion to alcohol
- Conversion to coal oil
- Conversion to electricity
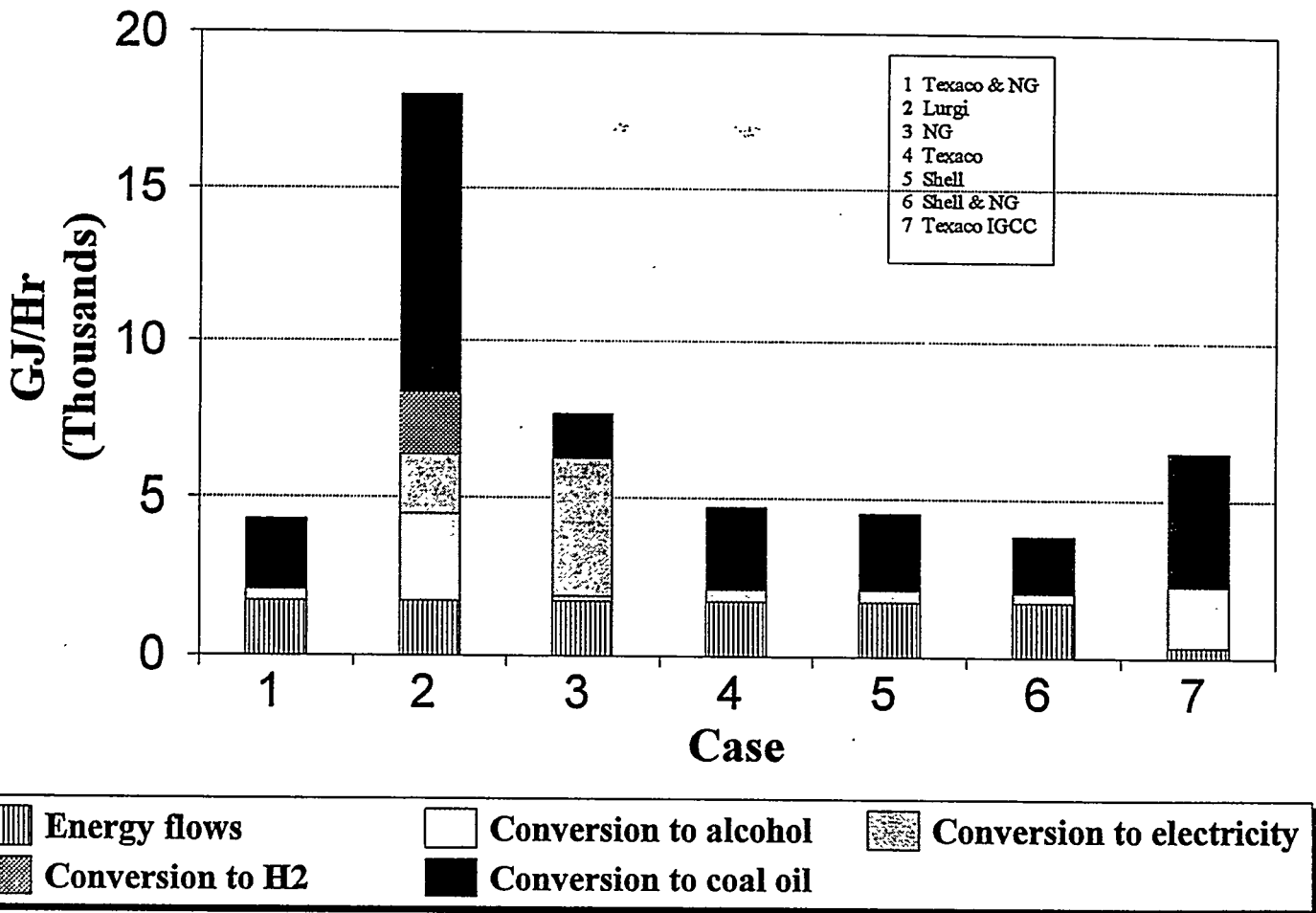
Table 6.3

Overall Energy Efficiencies and Distributions for Designs

Case	1	2	3	4	5	6	7
Energy Input GJ/hr							
Coal	3501.48	17994.19	0.00	4757.02	4593.03	2159.17	6417.04
Natural Gas	871.81	0.00	7670.86	0.00	0.00	1750.43	0.00
Total	4373.29	17994.19	7670.86	4757.02	4593.03	3909.60	6417.04
Energy Output GJ/hr							
Alcohol	1728.00	1728.00	1728.00	1728.00	1728.00	1728.00	345.76
Electricity	352.44	2808.00	150.12	375.12	374.40	302.40	1919.77
H2	0.00	1771.78	4289.32	0.00	0.00	0.00	0
Light Coal Oil Mix	0.00	2026.93	0.00	0.00	0.00	0.00	0
Total	2080.44	8334.72	6167.44	2103.12	2102.40	2030.40	2265.53
Losses	2292.84	9659.48	1503.42	2653.89	2490.63	1879.20	4151.51
Energy Flows							
conversion to alcohol	39.51%	9.60%	22.53%	36.33%	37.62%	44.20%	5.39%
conversion to electricity	8.06%	15.61%	1.96%	7.89%	8.15%	7.73%	29.92%
conversion to H2	0.00%	9.85%	55.92%	0.00%	0.00%	0.00%	0.00%
conversion to coal oil	0.00%	11.26%	0.00%	0.00%	0.00%	0.00%	0.00%
conversion loss	52.43%	53.68%	19.60%	55.79%	54.23%	48.07%	64.70%
TOTAL EFFICIENCY	47.57%	46.32%	80.40%	44.21%	45.77%	51.93%	35.30%

natural gas or produce the least amount of electric power. Of these processes, the steam reformation of natural gas (Case 3) yields the best overall efficiency assuming full credit is given to the energy contained as H_2. Closer examination of this process, however, reveals that only 22.5 percent of the total energy input actually goes to the production of alcohol. Given that the objective is to produce as much alcohol as possible, and that, at best, only half of the energy contained in H_2 can actually be recovered, Case 6 may provide better results. Case 6 has the highest efficiency with respect to alcohol conversion at 44.2 percent. However, the amount of natural gas consumed by these processes may impose a series of logistical problems if these facilities are located in remote areas not accessible to major natural gas distribution lines.

Confronted with these potential problems, it appears that one of the less efficient technologies, which relies entirely on coal, may ultimately provide a feasible solution. Case 5, which uses a Shell gasifier in conjunction with a sour gas shift converter, appears to be only slightly less efficient than its counterpart Case 6, which uses steam reformation of natural gas to increase the hydrogen content of the syngas. The difference between the overall efficiencies of these two cases is approximately 6 percentage points.

However, the most efficient case, by wide margin, is Case 3, which uses only natural gas. If pollution credits based on CO_2 or other combustion products are obtainable in the future, this process will benefit relative to the coal cases. The major question is whether an increase in natural gas prices would be completely offset by any potential gains realized by pollution credits.

6.3 Fugitive Emissions

To construct a plant such as the one being designed here, current environmental regulations must be followed, and anticipated environmental regulations must be considered. Therefore, a preliminary environmental analysis of the sulfur removal portion of Case 1, at the smallest scale, has been completed. This case includes fugitive emissions and stack emissions. The sulfur portion of the process is emphasized because all of the sulfur compounds along with a major part of the process's CO, volatile organic contaminants (VOCs) which are precursors to ozone formation, and two hazardous air pollutants (methanol and COs) are found in this portion of the process. The results indicate that, for SO_x compounds, there will be no trouble meeting environmental regulations. However, for reduced sulfur compounds (H_2S and COS) and for ozone producing VOCs, the process is over the current threshold values. This requires application of BACT (Best Available Control Technology) which could significantly increase the cost of construction and operation of a coal to syngas to higher alcohols process. Details of this analysis are in Appendix A.

7. Conclusions

- There are significant differences between the production costs for processes converting coal to syngas to higher alcohol fuel additives for cases involving Texaco, Lurgi, and Shell gasifiers, between cases involving natural gas reforming or sour gas shift conversion to alter the H_2/CO ratio, and for different plant capacities. The best case, on the basis of manufacturing cost, is one of the hybrids, a Shell gasifier with natural gas.

- Production of 5.1 billion liters/yr (32 MM bbl/yr) of alcohol fuels from coal is considered the maximum feasible process scale. As expected, there are economies of scale favoring larger-scale over smaller-scale processes. However, resource and marketing constraints limit the maximum scale at which a plant could be constructed.

- Production of higher alcohol fuel additives from natural gas is more economical, for the next 20 years, than production from coal at any scale at current or predicted (by DOE) natural gas prices. Production of higher alcohol fuel additives from coal and natural gas hybrids is more economical than production from natural gas at West Virginia natural gas prices ($3.00/MM BTU). The break even natural gas price for production of higher alcohols by natural gas versus the Shell gasifier/natural gas hybrid is $2.45/MM BTU. Furthermore, if a plant life of 10 years were used, which is more typical in the chemical process industry, then all of the manufacturing costs for the cases using coal gasification will increase, making natural gas the clearly superior option.

- Capital and operating costs are estimated on the basis of conventional technology, equipment, processes, and environmental controls. Thus, it is possible that future emission control requirements could significantly increase capital and operating costs of all coal-based processes described.

- The manufacturing cost of the alcohol derived from natural gas is highly dependent on the natural gas price. Capital costs are lower for natural gas cases than for coal-based cases. Therefore, raw material costs for the natural gas cases are a larger portion of the total annualized cost.

- If the cost of natural gas exceeds $2.45/MM BTU, the coal/natural gas hybrid (Shell gasifier) is more economical than the natural gas only design. If the cost of natural gas exceeds $4.94/MM BTU, the all coal design (Shell gasifier) is more economical than the hybrid. This is primarily a result of the high capital investment for the gasifier and accompanying cryogenic oxygen plant. This higher investment outweighs the benefit of using coal, which is a cheaper raw material. The only way for coal based processes to be more competitive than natural gas under all conditions is either for the relative price of coal and natural gas to change or for a major development to occur in coal gasification technology. Price variations would have greater impact on the natural gas reference cases, since raw material costs for these cases are a larger portion of the total

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annualized cost. Therefore, the competitiveness of the coal-based cases would be enhanced more by increases in the price of natural gas than by decreases in coal cost.

- The most energy efficient design, by wide margin, uses only natural gas. If pollution credits based on CO_2 or other combustion products are obtainable in the future, this process will benefit relative to the coal cases. The major question is whether an increase in natural gas prices would be completely offset by any potential gains realized by pollution credits.

8. Recommendations and Future Work

8.1 Optimization

A solution methodology to maximize the profitability of alcohol synthesis, separation, and blending has been developed. The temperatures, pressures, flowrates, and key component recoveries in the separation steps are the optimization variables. This methodology is robust and flexible; therefore, a wide-range of processing conditions can be investigated yielding consistent and accurate results. This methodology is in the process of being applied to the alcohol synthesis and separation portion of the process.

8.2 Sensitivity Analysis

8.2.1 Process

A methodology, using Monte Carlo simulation, to determine the effects and influences of process variable uncertainties on the performance of a design has been developed [22]. Input variables in the model to be considered include the reaction product distribution, the operating temperatures of equipment (e.g., gasifiers, separators, etc.), and the estimates in the thermodynamic model used in the computer aided design simulation of the process. The output variables are the manufacturing cost and the energy efficiency of the plant. Determination of the parameters that may cause uncertainty in the process will be accomplished by choosing those parameters that are probabilistic in value and those which are not correlated to other more significant parameters. The result will be a range of expected operating conditions for the process and an indication of which variables' uncertainties are most likely to affect process operating conditions.

8.2.2 Cost and Price

Costs and prices are not known with certainty, and the expected ranges may be sufficiently large to affect the relative rankings of the tested options as well as their absolute economics. In addition to the costs and prices of the inputs and outputs, prices of substitutes, such as MTBE and gasoline, also affect process economics. The relative expected growth rate in natural gas, oil, and coal prices determine the time in which coal-derived alcohol fuels may become economical.

To explore the effects that changing input and product prices have on the process economics, sensitivity analysis (Monte Carlo simulation) will be used. The results will indicate which processes have the most economic promise given the uncertainties of prices and costs.

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8.3 Energy Park

The potential exists for an integrated approach to produce mixed alcohols and energy (with an emphasis on electric power) given the various technologies currently under consideration. Each technology has its own strengths and weaknesses. By taking advantage of the strengths of these various technologies, the overall economics of alcohol production may be improved. This integration may be achieved in the context of an Energy Park, as described in Section 3.3. Future efforts will focus on taking advantage of this possibility.

8.4 Possible Additional Case Studies

The present results of this work indicate that a facility to produce higher alcohols for use as transportation fuel additives from coal is currently uneconomical. This situation may, of course, change if significant savings can be found in gasifier technology or if the price of natural gas increases significantly. Possible alternative processing schemes may be sought to identify potentially profitable alternatives in this area. Examples of alternative processing schemes include:

1. Economically disadvantaged feedstocks (EDF's) such as vacuum residuum and petroleum coke should be considered as potential substitutes for coal. The surplus of these refinery derived materials gives rise to a potential window of opportunity and may offset some of the economic disadvantages of solid-based feed materials.

2. The possibility of converting methanol (and other higher alcohols) to ethers via condensation type reactions should be considered. For example, dimethyl ether (DME) has potential as a diesel fuel additive [23].

Consideration may be given to such alternatives in the future.

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