

# The Economical Production of Alcohol Fuels from Coal-Derived Synthesis Gas

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## ABSTRACT

This program is dedicated to providing a cost effective process for converting coal-derived synthesis gas to liquid products useful as transportation fuels. One goal of this project is to develop and evaluate catalysts and reactors for the selective conversion of low hydrogen content syngas to alcohol fuel extenders and octane enhancers (Task 1). The target products are C<sub>2</sub>-C<sub>5</sub> alcohols, which can be used with methanol as gasoline octane enhancers. The second goal is the design of economical, energy efficient processes to convert coal to syngas and then to higher alcohols (Task 2). Energy integration, cogeneration, fuel testing, and economic uncertainty are also being investigated.

This report focuses on results from Task 2. Base case designs have been completed including Texaco and Shell gasifiers, with either natural gas or a sour gas shift converter to adjust the unfavorable H<sub>2</sub>/CO ratio exiting the gasifier. The alcohol synthesis reactor uses a MoS<sub>2</sub> catalyst and is of a shell and tube design previously proposed by Union Carbide Corporation. A comparison of the payback periods or production cost of these plants shows significant differences among the base cases. However, a natural gas only design, prepared for comparison purposes, gives a lower payback period or production cost. Since the alcohol synthesis portion of the above processes is the same, the best way to make coal-derived higher alcohols more attractive economically than natural gas-derived higher alcohols is by making coal-derived syngas less expensive than natural gas-derived syngas.

The maximum economically feasible capacity for a higher alcohol plant from coal-derived syngas appears to be 32 MM bbl/yr. This is based on consideration of regional coal supply in the eastern United States, coal transportation, and regional product demand. The benefits of economies of scale are illustrated for the base case designs.

A value for higher alcohol blends has been determined by appropriate combination of RVP, octane number, and oxygen content, using MTBE as a reference. This analysis suggests that the high RVP of methanol in combination with its high water solubility make higher alcohols more valuable than methanol.

In the future, the most attractive base cases will be used to determine optimum plant size and operating conditions. Tasks 1 and 2 will interact to determine catalyst and reactor operating conditions which produce the most appropriate product distribution under the most economical conditions. Simulated annealing, a technique especially suited for optimization involving discrete choices, will be employed. Monte Carlo simulations will be used to study process and economic uncertainties. Fuel testing will be done to evaluate the combustion, emission and performance characteristics of fuel alcohols and gasoline blends.

## **I. INTRODUCTION**

### **A. Organization**

This project is divided into two tasks. The objectives of Task 1 are in catalyst and reaction engineering. The objectives of Task 2 are in process synthesis and fuel evaluation. Interaction between these two tasks to facilitate selection of optimum catalyst properties and reactor operating conditions is essential. At this point, however, Task 2 is ahead of Task 1 because of delays in starting the experimental portion of the project due to the delay in obtaining government approval for the environmental consequences of the experimental program. Therefore, this paper focuses entirely on results from Task 2.

### **B. Goals**

The goals of this project are

- to discover, study, and evaluate novel heterogeneous catalytic systems for the production of oxygenated fuel enhancers from synthesis gas. Specifically, alternative methods of preparing catalysts will be investigated, and novel catalysts, including sulfur-tolerant ones, will be pursued. (Task 1)
- to explore, analytically and on the bench scale, novel reactor and process concepts for use in converting syngas to liquid fuel products. (Task 1)
- to simulate by computer the most energy efficient and economically efficient process for converting coal to energy, with primary focus on converting syngas to fuel alcohols. (Task 2)

- to develop on the bench scale the best holistic combination of chemistry, catalyst, reactor, and total process configuration integrated with the overall coal conversion process to achieve economic optimization for the conversion of syngas to liquid products within the framework of achieving the maximum cost effective transformation of coal to energy equivalents. (Tasks 1 and 2)
- to evaluate the combustion, emission and performance characteristics of fuel alcohols and blends of alcohols with petroleum-based fuels. (Task 2)

### C. Present Work

This report is focused on the results obtained by Task 2. Base Case designs have been developed involving alternative syngas production processes with identical alcohol synthesis modules. Identical processes of different scale have also been evaluated. These processes are all compared in terms of the price of oxygenate fuel additive vs. payback period for capital investment and in terms of the production cost of oxygenate product.

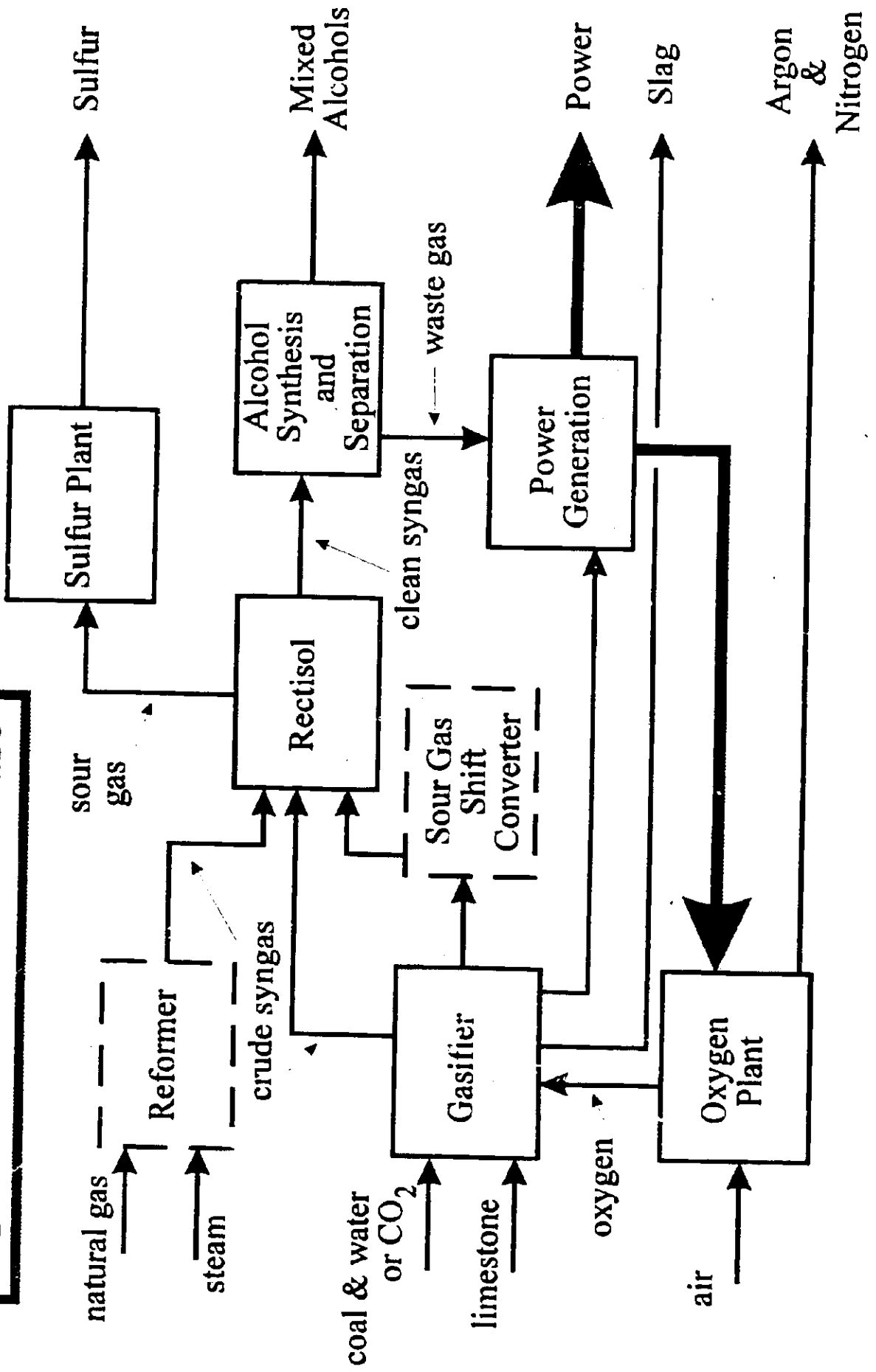
## II. METHODOLOGY

### A. Process Concept

A generic process for converting coal to syngas to higher alcohol fuel additives is outlined in Figure 1. The oxygen plant provides oxygen for the gasifier. The sour gas shift converter adjusts the  $H_2/CO$  ratio to the desired ratio of 1.1/1 using the water gas shift reaction,  $CO + H_2O \rightarrow CO_2 + H_2$ , with the necessary steam provided by vaporization of water used to slurry the coal. An alternative process might employ steam reforming of natural gas,  $CH_4 + H_2O \rightarrow CO + 3H_2$ , to adjust this ratio. Acid gas treatment and sulfur removal precede alcohol synthesis. A portion of the syngas is split from the gasifier effluent and sent to a power plant to generate at least as much power as is needed by the rest of the plant. The alcohol synthesis reactor is assumed to be a shell-and-tube design with the  $MoS_2$  catalyst in the shell. Use of the  $MoS_2$  catalyst yields a product that is primarily  $C_1$ - $C_5$  linear alcohols.

For the initial base case designs, one unit train of coal ( $\approx 10^4$  tons) per week (1400 tons/day), was assumed. This is about 7-8 times less than the amount of coal used by a typical full-scale power plant, and a reasonable minimum size plant to consider. For the purposes of discussion, we are assuming that this coal to alcohol fuels plant would be located somewhere in southern West Virginia. If these initial base case designs were scaled-up by a factor of 8, 32 MM bbl/year of alcohol fuel additive would be produced, which is about 10% of the total gasoline sold in a seven state area surrounding West Virginia. This scale seems a reasonable upper limit on plant size if the alcohol fuel is to be used as an additive comprising <10 vol % in gasoline. Finally, assuming the same plant location, 8 unit trains of coal per week represents the output of three of the largest mines

**Figure 1: Generic Base Case**



in West Virginia. The facility must be located near mines of this size so that transportation costs do not inflate the cost of coal so much that the alcohol fuel becomes too expensive.

## B. Target Blends

To provide a production goal for the designs, target products are necessary. All fuels for light-duty gasoline vehicles must be certified by EPA. Two blends already certified (i.e., granted waivers) that are closest to our projected product are the DuPont blend (1,2) and OCTAMIX™ (3). These blends contain <5 vol % methanol and >2.5 vol % higher alcohols (C<sub>2</sub>-C<sub>4</sub> for DuPont, C<sub>2</sub>-C<sub>8</sub> for OCTAMIX™) plus 40 mg/L of a corrosion inhibitor necessitated because water is soluble enough in methanol to corrode automobile gasoline distribution systems. The products to be developed in this project are similar to these blends. For these blends, little or no purification of the alcohol synthesis reactor product is necessary.

## C. Economics

Equipment costs were obtained from previous designs (4-8). Costs were assigned to a module (e.g., Rectisol) rather than by evaluating each piece of equipment within the module. To determine the appropriate cost for a module of the desired size, an exponential scale factor was found by regressing all available designs of different size. Extrapolation beyond the limits of the data was used, if necessary. For the cases in which only a single point was available, a scale exponent of 0.7 was used.

The prices assumed for reactants, products and by-products are shown in Table 1. It was assumed that all by-products such as sulfur and slag could be sold at the indicated price.

<b>Item</b>	<b>Price</b>
Coal	\$33/metric ton delivered
Power	\$0.05/kw-hr
Slag	\$5.5/metric ton
Sulfur	\$300/metric ton
Natural Gas	\$100/1000 std m <sup>3</sup>

No price is indicated for the alcohol fuel product. Instead, the cost of production of the product was calculated for various pay back periods.

## D. Scale-up Methods

To scale-up the initial base cases, exponential and linear scaling was used as appropriate. Individual pieces of equipment or modules were scaled exponentially. If data on different size modules or equipment were available, the data were used to determine the scale factor. If insufficient data were available, an exponential scaling factor of 0.7 was used. However, maximum sizes for modules and especially for the gasifiers were determined from previous studies. When a maximum size was reached, parallel trains were added to achieve the desired scale, hence, linear scaling.

## III. RESULTS AND DISCUSSION

### A. Base Case Designs

Six base case designs have been completed. Their features are shown in Table 2.

<b>Base Case Number</b>	<b>Gasifier</b>	<b>H<sub>2</sub>/CO adjustment</b>
1	Texaco	steam reforming of natural gas
2	Lurgi	steam reforming of natural gas
3	None (Natural Gas only)	PSA to separate excess H <sub>2</sub>
4	Texaco	sour gas shift converter
5	Shell	sour gas shift converter
6	Shell	steam reforming of natural gas

The rationale for choosing these cases is as follows. The Texaco and Shell gasifiers are modern, entrained bed gasifiers operating at high temperatures and produce no unwanted by-products. The Lurgi gasifier is old technology, operates at lower temperatures, and produces phenolic and related by-products. The reason for including this base case is to

investigate whether there is any economic advantage to producing these by-products. As will be seen later, there is no advantage to this alternative, even under the assumption that 100% of the by-products generated can be sold. Therefore, this case has not been pursued any further. Base Case 3, natural gas only, is included for comparison only, since the stated goal of this research is to use coal as the raw material. It will be shown, however, that this base case produces the least expensive product, at current prices. Therefore, the combined coal/natural gas cases were also included.

Figures 2 and 3 illustrate Base Cases 1 and 5, respectively. Base cases 4 and 6 can be obtained from 1 and 5, respectively, by exchanging the steam reforming and sour gas shift conversion modules, and are not illustrated. Base Case 3 is shown in Figure 4. Pressure swing adsorption is used to separate excess hydrogen to reach the desired  $H_2/CO$  ratio of 1.1/1.

The reasons for selecting specific modules is as follows. Cryogenic oxygen separation is superior to pressure swing adsorption or membranes for the scale of these separations. Rectisol is chosen because it is a popular acid gas treatment process, and it works for the current configuration. UCarSol, a proprietary Union Carbide solvent process, does not work due to a "temperature bulge." This means that heat generated by the exothermic adsorption of acid gases makes the adsorption equilibrium unfavorable. The Selexol process is still being studied. While there are more alternatives, there is a paucity of cost information for these (e.g. hot potassium carbonate). The Claus and Beavon processes are chosen for sulfur removal because they are proven technology. While there are alternatives, the cost of these modules is very small compared to the cost of the entire process; hence, there is little benefit to investigating alternatives. The alcohol synthesis reactor using a  $MoS_2$  catalyst and producing linear  $C_1-C_5$  alcohols is chosen because there is information available on a product distribution and reactor cost as a function of size.

In all of the base case designs, about 10% of the hot gases generated from the gasifiers (except base case 3) and light gases separated from the alcohol synthesis reactor effluent (all base cases) are used to generate power. Additionally, in the coal base cases, steam produced by recovering heat from the gasifier outlet is also used to generate power. The amount of power generated is slightly greater than that consumed in the remainder of the process. In future optimization studies, the consequences of generating more power at the expense of producing alcohol fuels will be investigated.

Figure 5 shows the cost of production of the alcohol fuel product as a function of payback period for the six base cases. All of the coal base cases give similar results. However, it is clear that, at current prices, natural gas is a superior choice. The two natural gas cases, 3 and 3H, assume no credit and \$1.74/1000  $ft^3$  (merchant grade) credit for hydrogen, respectively. Since the market for excess hydrogen is unclear, these two cases represent the two extremes. An alternative use for hydrogen would be internally as a fuel.

Figure 2: BASE CASE #1

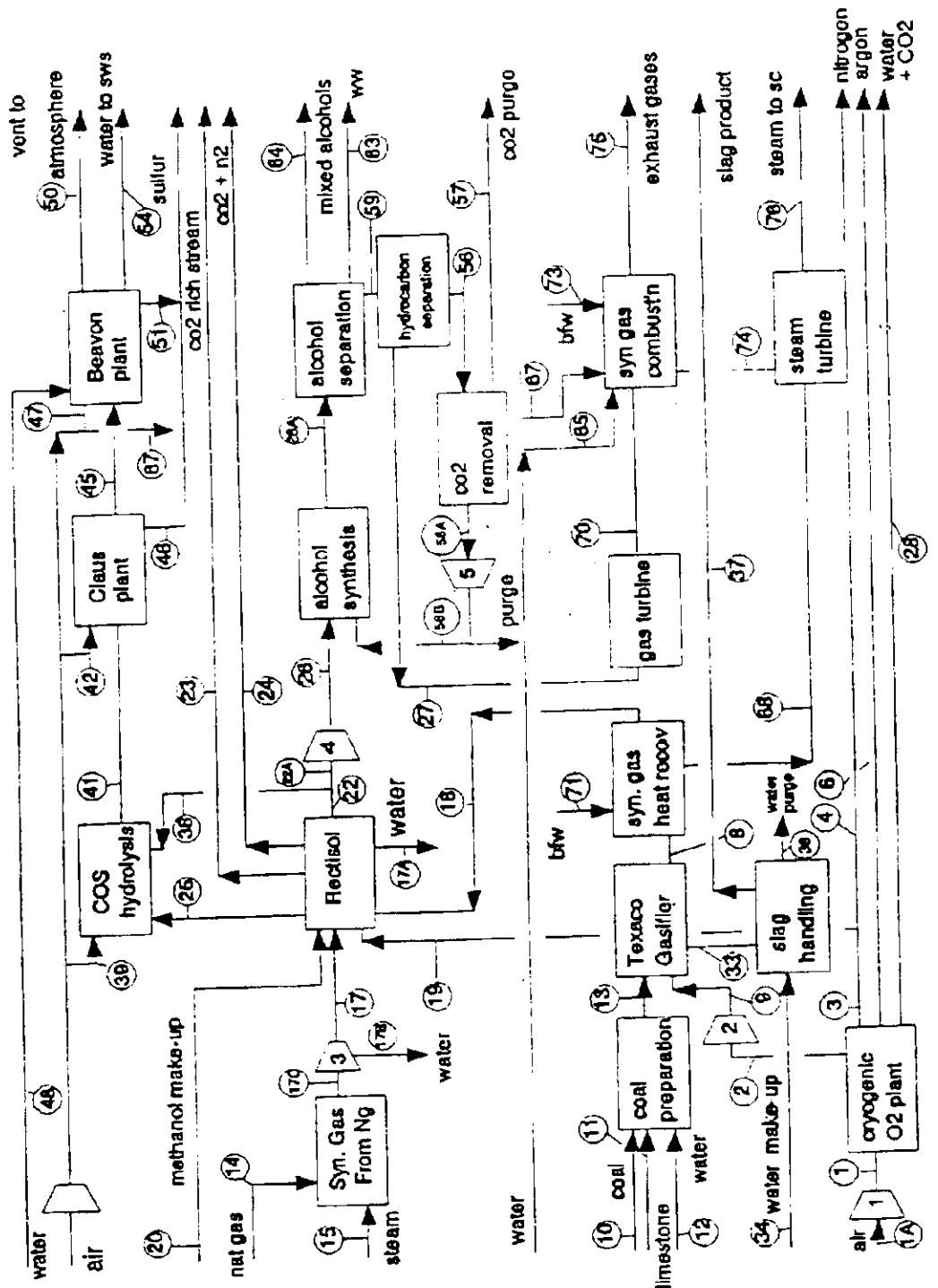
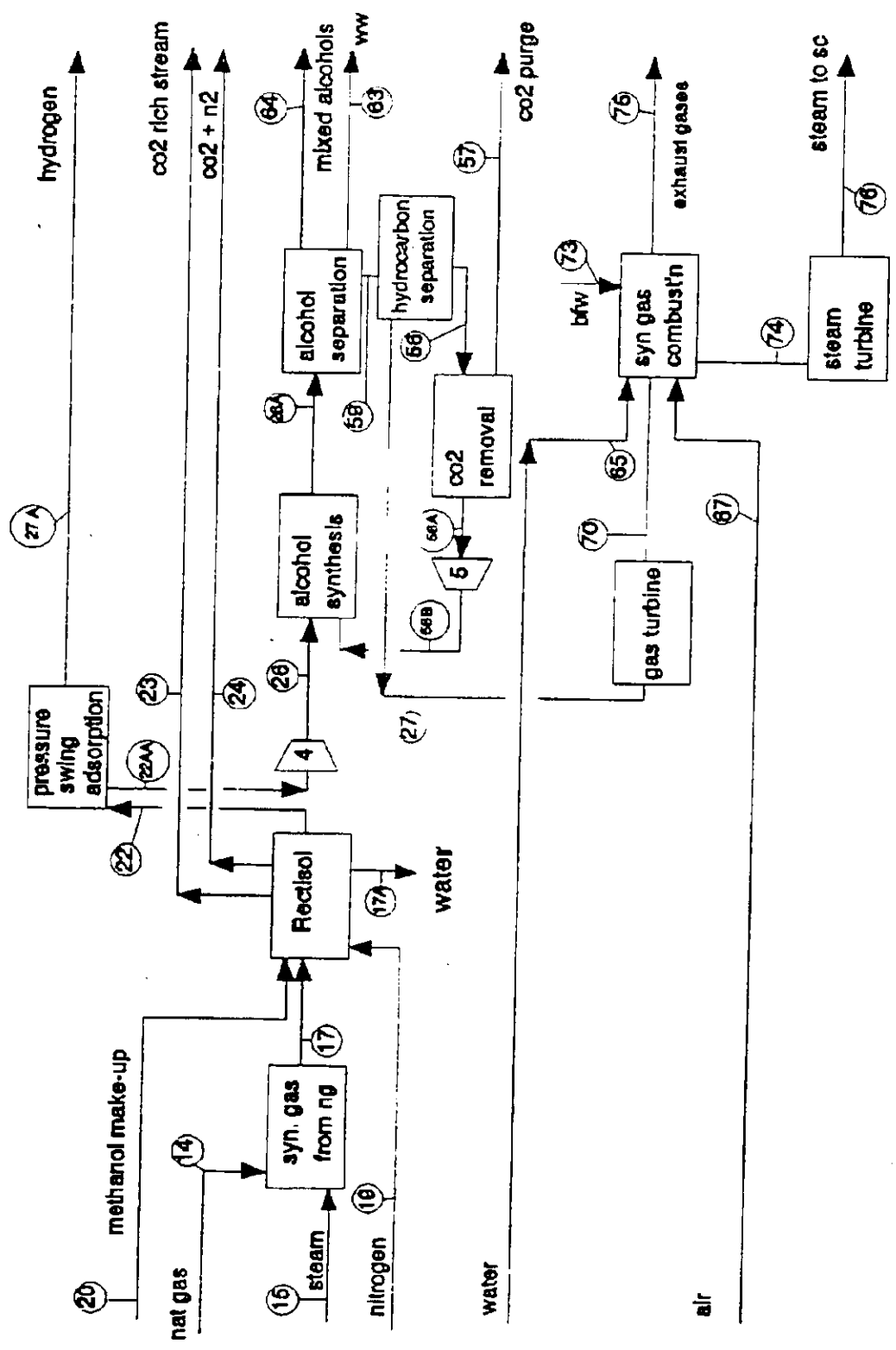


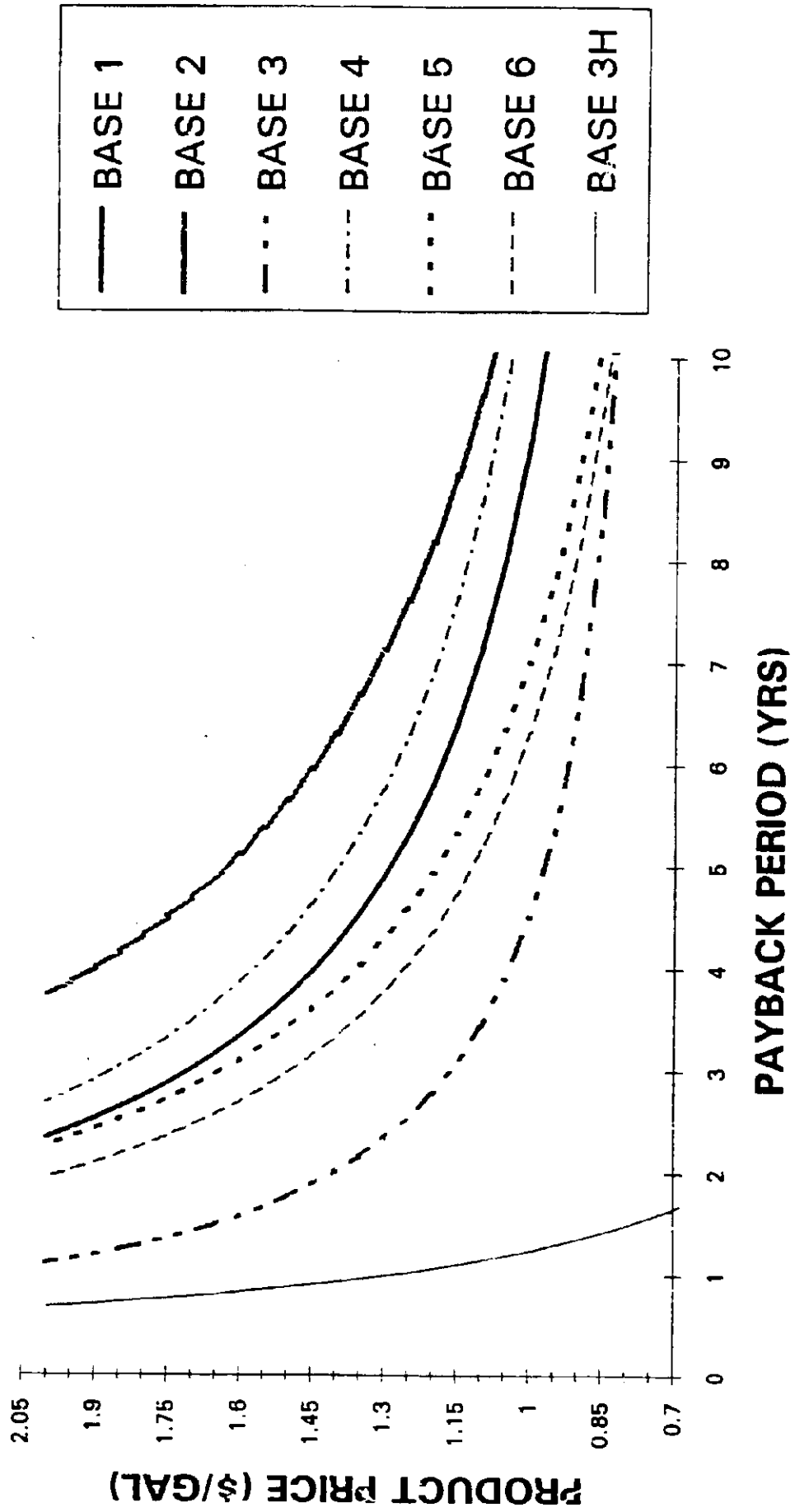




Figure 4: BASE CASE # 3



**FIGURE 5: PAYBACK PERIOD FOR BASE CASES**



## B. Sample Results

To provide some insight into the origin of Figure 5, more detailed results for Base Case 1 are presented. Table 3 contains an itemized list of the capital investment. Table 4 contains a summary of capital costs, annual operating costs, and by-product credits for all base cases at all scales. For the initial comparison to date, we use pay back period, which is a simple, before-tax method, without adjustment for the time value of money. For example, a pay back period of 8.5 years corresponds to a before-tax discounted cash flow rate of return (DCFROR) of approximately 10% for a plant life of 20 years. The costs are indexed to 1992, and inflation is not considered.

<b>Module</b>	<b>Cost (MMS)</b>
Steam Reforming	15.9
Coal Preparation	43.1
Texasco Gasifier	117.5
Slag Handling	2.7
Steam/Power Generation	109.5
Synthesis Gas Heat Recovery	4.1
Cryogenic Oxygen Production	80.0
Rectisol (Acid Gas Separation)	33.3
COS Hydrolysis	-
Claus (Sulfur Recovery)	9.2
Beavon (Final Sulfur Removal)	2.0
Alcohol Synthesis (MoS <sub>2</sub> Reactor and Separation System)	46.9
CO <sub>2</sub> Removal in Alcohol Synthesis Loop	31.3
Other Compressors	37.3
<b>TOTAL</b>	<b>532.8</b>

**Table 4**  
**Summary of Costs for Base Cases**

<b>Base Case</b>	<b>Alcohol Production (MM bbl/yr)</b>	<b>Capital Cost (MMS)</b>	<b>Operating Cost (MMS/yr)</b>	<b>By-Product Credits (MMS/yr)</b>
1	4	532.8	133.9	22.2
	8	955.3	267.8	44.4
	16	1,757.8	535.6	88.8
	32	3,291.6	1,071.2	177.6
2	4	931.5	236.9	146.6
	8	1,734.3	473.8	293.2
	16	3,276.7	947.6	586.4
	32	6,212.3	1895.2	1,172.8
3	4	248.3	144.5	29.5
	8	409.2	289.0	59.0
	16	691.4	578.0	118.0
	32	1,191.7	1156.0	236.0
3H	4	248.3	144.5	175.0
4	4	600.8	135.6	18.8
	8	1,062.7	271.2	37.6
	16	1,981.4	542.4	75.2
	32	3,713.0	1,084.8	150.4
5	4	568.6	132.8	44.0
	8	975.2	265.6	88.0
	16	1,822.3	531.2	176.0
	32	3,398.9	1,062.4	352.0
6	4	484.0	123.9	30.0
	8	832.4	247.8	60.0
	16	1,418.6	495.6	120.0
	32	2,556.4	991.2	240.0

## C. Natural Gas vs. Coal

It is clear from Figure 5 that natural gas is superior to coal as a source of alcohol fuels if excess hydrogen can be sold or used internally as a fuel. The reason for this is illustrated in Figure 6. The alcohol synthesis module is identical in all of the base cases. The difference between the natural gas base case and the coal base cases is the "front end." The cost of producing syngas from coal is currently much greater than producing it from natural gas if excess hydrogen can be sold or used internally. The only way for coal to be more competitive under all conditions is for the relative prices of coal and natural gas to change or for a major development in coal gasification technology to reduce the cost for producing coal-derived syngas. An examination of Figure 5 shows that, at a mixed alcohol fuel additive price of \$1.03/gal (see Table 5 and Section IV.A.1), the best payback period for coal derived product is about 6.5 years, which is equivalent to a 14% ROI, based on a plant life of 20 years, without considering the effects of inflation or taxes.

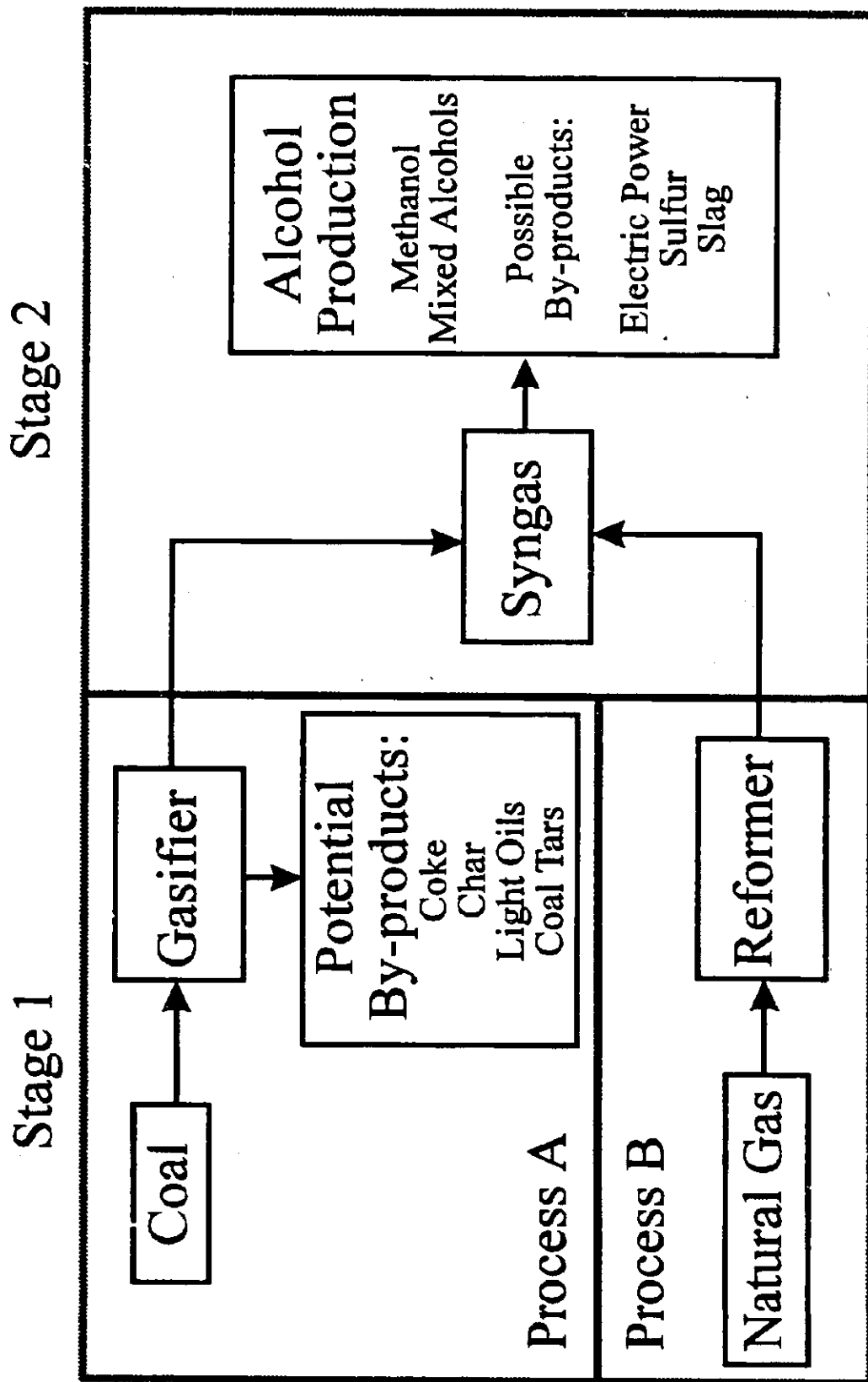
## D. Scale-up

Figure 7 shows the impact of plant capacity on production cost. An increase in plant capacity makes a Shell gasifier with natural gas the most attractive case. Furthermore, the economic advantages of a Shell gasifier over a Texaco or Lurgi gasifier are clear. There are also economies of scale; however, they diminish above a 32 MM bbl/yr plant capacity. The plant gate costs in Figure 7 represent a 10% return of capital over a 20 year plant life without considering the effects of taxes or inflation.

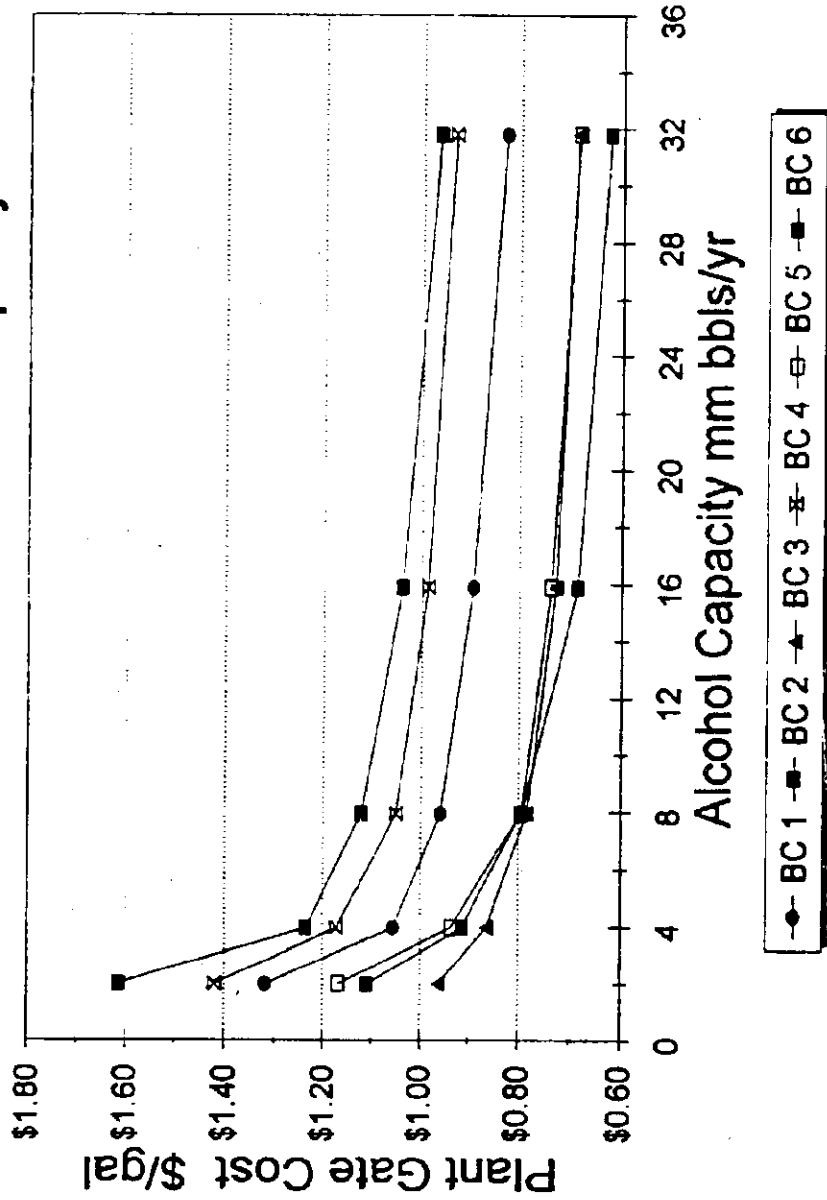
## E. Fugitive Emissions

To construct a plant such as the one being designed here, current environmental regulations must be followed. Therefore, a preliminary environmental analysis of the sulfur removal portion of Base Case 1, prior to scale-up, has been completed. This 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, 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<sub>x</sub> compounds, there is no trouble meeting environmental regulations. However, for reduced sulfur compounds (H<sub>2</sub>S and COS) and for ozone producing VOCs, the process is over the 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.

Figure 6: Alternative Syngas and Alcohol Production Pathways



**Figure 7:**  
**MIXED ALCOHOL FUELS**  
**Gate Cost as a Function of Capacity**





## IV. WORK IN PROGRESS AND FUTURE WORK

### A. Optimization

#### 1. Overview

With the base cases for different process configurations at different scales complete, the focus of this project now turns toward optimization. To optimize any process, a suitable objective function is required. To generate such a function, such as equivalent annual operating cost (EAOC) or DCFROR, a value must be assigned to the price of the alcohol fuel product. Since there is no current market for this product, assumptions must be made.

A method using MTBE as a reference is being used to assign values to higher alcohol fuel products. The method is based upon RVP, octane number and oxygen content, and has been used previously to determine the value of ether fuel additives (9). The results are presented in Table 5. With these values available, it is now possible to generate an objective function to optimize the alcohol synthesis portion of the process. Optimization procedures are outlined below.

**Table 5**  
**Estimated Value of Alcohol Fuel Additives**

<b>Component</b>	<b>Blending Value (\$/gal)</b>
methanol	0.98
ethanol	1.13
propanol	0.91
butanol	0.86
pentanol	0.83
mixed alcohol product*	1.03
MTBE	0.95

\*value obtained based upon base case product distribution  
from alcohol synthesis reactor

#### 2. Simulated Annealing

Simulated annealing is an algorithm for single objective, multi-variable optimization problems. It draws an analogy between the minimization of energy achieved by annealing a physical system and the minimization of a cost function required in optimization (10). Simulated annealing asymptotically converges to a global optimal solution to every combinatorial optimization problem under the limiting condition of infinite computation

time. However, in realistic situations, it is the finite time behavior, i.e., the use of simulated annealing as an approximate algorithm which is of greater interest (11). As an approximate algorithm, simulated annealing provides near-optimal solutions in polynomial time to exponential time problems. The algorithm for simulated annealing consists of repeatedly making a move to change system configuration and accepting or rejecting the move based upon an acceptance probability, while periodically reducing the "annealing temperature." (12) The algorithm is made to terminate when a specified criterion is satisfied.

Simulated annealing is particularly well-suited to optimization of processes involving discrete choices. In fact, simpler optimization procedures are easier to use for processes involving continuous functions. In the current process, when choices such as Texaco or Shell gasifier must be made, simulated annealing is the best optimization procedure available. To date, simulated annealing has never been applied to optimization of an entire process such as the one involved here.

The optimization of a process flow sheet can be treated as a single objective optimization problem with a large number of variables. A function of the total installed and operating cost, such as EAOC and DCFROR, can be considered as the objective function. Process conditions such as pressure, temperature, flow rates, etc., can be considered as variables.

It is very inefficient to compute a new cost for each process configuration encountered. Therefore, as a simplification, the cost of each piece of equipment is calculated over a wide range of process conditions and flow rates; and, the data generated are fit to an equation for inclusion in the objective function. The data are generated using Aspen Plus™.

While there are no results available yet, the methodology appears to be working. The delay is due to the time needed to generate the components of the objective function described in the previous paragraph. Initially, the alcohol synthesis and separation portion of the process will be optimized. Ultimately, simulated annealing will be applied to the entire process.

### **3. Monte Carlo Simulation**

In simulation and optimization of a complex process, such as coal to alcohol fuel, there are always uncertainties in the data used. Physical properties of complex mixtures are assumed based upon pure component properties. Costs for raw materials and products are assumed based upon current values and current regulations. There are uncertainties in the physical properties and economic or political factors that could affect the price of raw materials or products.

Monte Carlo simulation can be used to determine the effect of these uncertainties on the process and can also be used to optimize the process in the face of these

uncertainties. It is well-suited for studies of systems with many uncertain process and simulation inputs, especially when these uncertainties produce nonlinear perturbations of the system.

Random values of uncertain parameters are chosen, based on their estimated statistical frequencies. An efficient stratified sampling technique known as Latin Hypercube Sampling is used to sample all important regions without bias. The results of the Monte Carlo simulation produce a ranking of the most important uncertainties as well as frequency distributions for process performance variables. We thereby quantify safety factors and process flexibility as well as estimate the probability of successful future economic performance.

We have previously used Monte Carlo techniques for economic forecasting, process-sensitivity evaluation, and optimization (13). We shall apply these techniques to the entire process.

#### **4. Heat Integration**

Given the large temperature changes within the coal to alcohol fuels process, there are certainly opportunities for heat integration. One method for performing heat integration is the use of pinch technology. The program ADVENT™ (ASPEN Tech) has been developed especially for this purpose. As part of process optimization, process heat integration will be investigated. This work will be performed at Union Carbide Corporation.

### **B. Energy Park**

The efficient utilization of coal reserves is anticipated to grow in importance as energy requirements increase and oil recovery slows. A holistic approach, which we call the *Energy Park* concept, would appear to be an important factor in efficient energy usage.

By definition, an energy park is a combination of facilities that utilizes one or more types of fuel in one or more types of conversion technologies to produce more than one product with the goal of reducing costs through the production of by-products, increased energy efficiency, and reduced pollution. The technologies, fuel and pollution problems related to producing coal-based alcohol fuels are highly amenable to being included in an energy park. This means all types of fuels, including coal and natural gas, should be considered as inputs. The use of natural gas along with coal in Base Cases 1 and 6 is an example of this. Also, more than one type of technology, including high and low temperature gasification, should be considered. In addition, the co-production of power, alcohol fuel, coal chemicals, and useful steam must be considered as a means to increase energy utilization efficiencies and to decrease overall costs.

We plan to use the process synthesis and optimization methods described above to evaluate a spectrum of possibilities for turning coal into energy or chemical feed stocks. Examples might include cogeneration of syngas for fuel alcohols, acetylene, high grade coke for electrodes, fly ash for building materials, along with steam and electricity. This is one reason for including the base cases with natural gas, because it may be more energy efficient to use natural gas to increase the H<sub>2</sub>/CO ratio of the syngas.

As part of the optimization process, we will evaluate how to recover the maximum value (products and energy) from an integrated conversion of coal to energy sources. Integrating coal combustion, syngas production, low grade heat recovery, and possibly chemicals production, should allow us to arrive at increased overall utilization of energy as well as of carbon and hydrogen.

### **C. Fuel Evaluation**

Of the various options available to the automobile industry, only alcohols appear to have possibility of being phased into use in the existing conventional automobile population. However, alcohols and especially the higher alcohols have been more expensive than gasoline and hence, have not gained much large scale attention as a primary energy source in the United States. The fuels evaluation component is aimed at evaluating fuel alcohols typical of those generated by the catalysts being studied in this research effort. The combustion and emission characteristics of the gasoline-alcohol blends will be evaluated.

Oxygenated fuels differ from gasoline and between themselves with regard to octane rating, water tolerance, exhaust emissions, corrosiveness, volatility and fuel economy. While abundant information is available in the published literature on the characteristics of methanol and ethanol blends with gasoline, data on higher alcohols blends with gasoline are lacking. The initial phase of this study was directed on a literature search on the state-of-the art in higher alcohols, both as neat and blended fuels. Based on the total oxygen content of the final product, RVP, methanol content, and octane number a series of blend compositions have been obtained. These potential blends in addition to the blends from the base cases developed in Task 1 will be chemically characterized for octane number, specific gravity, API gravity, sulfur content, flash point, viscosity, aromatic and olefin content, RVP and the distillation points. The chemical characterization is being conducted by certified labs. The combustion and emission characteristics of the fuels will be evaluated in the WVU Engine Research Center (ERC). A single cylinder Waukesha Cooperative Fuel Research (CFR) engine will be operated in steady state modes using the test blends. The single cylinder engine can be operated over a range of speeds and loading conditions and the compression ratio can be varied along with spark timing. The engine is equipped with standard instrumentation for on-line measurement of crank angle position, temperatures, in-cylinder pressure, fuel and air flow rates and exhaust emissions. Figure 8 shows a schematic of the engine test apparatus. The exhaust emissions will be sampled, for the steady state cases, using a total exhaust constant volume sampler (CVS) that was

constructed for the CFR engine. The bag samples will be analyzed for carbon monoxide, oxides of nitrogen, total hydrocarbons and carbon dioxide using Rosemount exhaust gas analysis equipment. Aldehydes and unburned alcohols will be sampled through 2,4-DNPH (dinitrophenyl hydrazine) coated silica gel cartridges and deionized water bubblers, respectively.

A comparison of the results, from the combustion and emissions tests, with those for conventional fuels will allow a meaningful evaluation to be made of the fuel characteristics concerning the potential of alcohol-gasoline fuel blends derived from coal.

#### **D. Interaction between Task 1 and Task 2**

Eventually, there will be significant interactions between Tasks 1 and 2. It is anticipated that process optimization will involve selection of the best catalyst properties and reactor operating conditions to maximize (or minimize) the objective function. However, realistic physical constraints exist. As Task 1 learns more about catalyst properties and reactor behavior, Task 2 will be able to incorporate this information into optimization models. Similarly, the results of optimization studies will yield suggested operating conditions for minimum cost, and it will be the goal of Task 1 to determine whether these operating conditions are feasible and reasonable.

### **V. CONCLUSIONS**

- There are significant differences between the payback periods and 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.
- Production of 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, there appear to be diminishing economies of scale above this plant size.
- A reasonable price for mixed alcohol product is \$1.03/gal, which is calculated by comparison of appropriate properties relative to MTBE. At this price, the estimated best case payback period is for a Shell gasifier with natural gas and is 6.5 years, which corresponds to a return on investment of 14%, without consideration of taxes and inflation.
- Production of higher alcohol fuel additives from natural gas is more economical at any scale at current or predicted natural gas prices if excess hydrogen can be sold or used internally as a fuel. For a 10% discount rate, at 4 MM bbl/yr, natural gas is more economical even if excess hydrogen is assumed to have no value.

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