

# Chapter 9

## Methodology

### 9.1 Design

#### 9.1.1 Case Studies

There were seven case studies developed in this work, which are presented in this report. Each of the first six case studies uses a different front-end configuration of process blocks to produce essentially the same amount of synthesis gas feed, with the same composition, to the alcohol production block. The mixed alcohol product is the same for each of the cases. The main difference between the case studies lies in what material is used as the source of the carbon and hydrogen for the synthesis gas production. Cases 4 and 5 use only coal as the raw material, and each case uses a different gasifier. Cases 1 and 6 use a mixture of coal and natural gas as the raw material, with each case using a different gasifier. Case 7 is a power production facility with a base-load of 500 MW and a peaking load of 100 MW for two two-hour periods per day, with higher alcohols produced as by-products. The peaking power is produced by burning methanol produced in the synthesis reactor, with the higher alcohols sold as fuel additives. For all these cases, we assume a Pittsburgh coal. Case 3 uses natural gas only and serves as a baseline economic comparison for the other cases. Two subcases are considered. For Case 3A, we assume a natural gas cost of \$106/1000 std m<sup>3</sup>. For Case 3B, we assume \$61.8/1000 std m<sup>3</sup>. The cost used in Case 3A represents a typical industrial natural gas price in West Virginia. The Case 3B cost is the corresponding Gulf Coast price.

The optimal synthesis gas feed to a process to produce C-1 and higher alcohols should contain a hydrogen to carbon monoxide ratio ( $H_2/CO$ ) of 1.1/1 [6, 7]. Since neither coal nor natural gas can be used directly to produce a synthesis gas with this  $H_2/CO$  ratio, additional processing of the gas is required. Two basic approaches were taken in this regard when considering coal. The first approach was to supplement the hydrogen-deficient synthesis gas from a coal gasifier with the hydrogen-rich gas produced by reforming natural gas. By adjusting the ratio of coal and natural gas feeds to the plant, the desired composition and flow of synthesis gas was produced by directly blending the cleaned gases from both processes. The second approach was to adjust the  $H_2/CO$  ratio of the gas produced in the coal gasifier by shifting some of the carbon monoxide to carbon dioxide via the water-gas shift reaction:  $CO + H_2O \leftrightarrow CO_2 + H_2$ .

This second approach has the disadvantage of requiring a much larger coal feed and hence requires larger (or more) gasifiers to produce the required amount of synthesis gas. In Case 3 the synthesis gas is produced by the steam reformation of natural gas followed by the removal of excess hydrogen via pressure swing adsorption. The relative benefits and economic potentials of each of these cases are considered further in Section 5.

### 9.1.2 Scale of Operation

The choice of the size of plant to be considered depended upon a combination of process and economic constraints. Upper and lower bounds on the size of the production facility were set using the rationale outlined below.

The lower bound on the size of the production facility was set by considering economically reasonable lower bounds on both coal and oxygen feed rates to the plant. Since the main thrust of this work was to concentrate on the gasification of coal to produce synthesis gas, it was decided to focus mainly on modern oxygen-blown gasifiers such as the Texaco and Shell processes. A reasonable lower bound on coal feed was considered to be one unit train of coal (~9100 metric tons (10,000 tons)) per week (1270 metric tons/day, 1400 tons/day). We used cryogenic separation of air, since this is the best way to produce the corresponding quantities (~2000 metric tons/day) of high purity oxygen [8]. For the purposes of discussion, we are assuming that this coal-to-alcohol-fuels plant would be located in southern West Virginia.

If the minimum sized plant were scaled-up by a factor of eight, 5.1 billion liters/yr (32 MM bbl/yr) of alcohol fuel additive would be produced, which is about 8% 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, for most cases, this limit resulted in plant scales up to 20 unit trains of coal per week (about 10 million tons/year). This represents the output of three of the largest mines in West Virginia. The coal supply pattern also indicates that this is a maximum size of plant. The facility must be located near mines of this size so that transportation costs do not significantly increase the delivered cost of coal to the alcohol plant. Because it uses more coal per unit of alcohol product, Case 2 reaches this coal constraint at a higher alcohol production rate of only 2.5 billion liter/yr (16 MM bbl/yr).

There are also limits to plant size because of natural gas supply limitations. Case 6, for example, uses approximately 220 million standard cubic meters (7.8 billion cubic feet) of natural gas a year to produce approximately 640 million liters/yr (4 MM bbl/yr) of alcohol. This is equivalent to roughly 16 percent of the industrial gas consumption for the state of West Virginia. If this facility's capacity is increased by a factor of eight, the amount of natural gas consumed by this facility would be equivalent to approximately 60 percent of the *total* natural gas consumption of this state. The possibility of supplementing commercial natural gas with coal bed methane in West Virginia was examined as a means of circumventing this potential constraint. Since there are no reliable statistics on coal bed methane reserves for West Virginia, an estimate was made using different sources of data [9, 10]. Although there appear to be sufficient reserves to meet the requirements of the proposed facility, collection and quality problems overshadow any potential benefits that coal bed methane may offer.

Since large scale facilities using steam reformation of natural gas for the production of syngas, such as Case 3A at x4 and x8 scales, would not be feasible for this region, an

alternative natural gas case (Case 3B) has been added for comparison purposes. Case 3B uses the same process design as Case 3A; however, it assumes a lower natural gas price that would be indicative of regions capable of supplying large quantities of natural gas on contract to a facility of this nature.

### **9.1.3 Available Technology**

The rationale for selecting specific process modules is as follows. The choice of modern, efficient, oxygen-blown gasifiers (Shell and Texaco) was addressed previously. A Lurgi gasifier was also used in one case (Case 2) in an attempt to produce a suite of profitable coal-liquid by-products. This approach proved to be economically unattractive and was not pursued further.

Cryogenic oxygen separation was preferred to pressure swing adsorption or membrane separation because of the large scale of oxygen production required for this process. Rectisol was chosen because of its wide-spread use in the removal of acid gases from coal-derived synthesis gas. UCarSol, a proprietary Union Carbide solvent process, was also considered. However, this process does not work because of a “temperature bulge” caused by heat generated in the exothermic absorption of acid gases leading to unfavorable equilibrium conditions for the absorption. The Claus and Beavon processes were chosen for sulfur removal because they are proven technologies. While there are alternatives, the costs of these modules are very small compared to the cost of the entire process; hence, there is little benefit to investigating alternatives.

The alcohol synthesis reactor using an  $\text{MoS}_2$  catalyst and producing linear  $\text{C}_1$ - $\text{C}_5$  alcohols was chosen because of the published information available on product distributions [7] and reactor costs and because Task 1 of this project is focused on developing novel  $\text{MoS}_2$  catalysts.

## **9.2 Economics**

### **9.2.1 Assumptions**

Equipment costs were obtained from previous designs [6, 7, 11-13]. 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, exponential scaling was used within a train, and linear scaling was used for multiple trains.

The prices assumed for reactants, products, and by-products are shown in Table 4.2. It was assumed that all by-products such as sulfur and slag could be sold at the indicated price.

A method using MTBE as a reference was used to assign values to higher alcohol fuel products. The method is based upon RVP and octane number, and a similar method has been used previously to determine the value of other fuel additives [14]. The results are presented in Table 4.3. The value of unleaded gasoline {50 kPa (7.2 psia) RVP, 87 octane ((RON+MON)/2)} was chosen as \$0.170/liter (\$0.644/gal). N-butane was valued at \$0.085/liter (\$0.321/gal), and MTBE was valued at \$0.223/L (\$0.845/gal). These values are the means of the weekly spot prices during 1992 [15, 16]. The relationship used was

$$value(\$ / L) = 0.023 - 0.0037(RVP \text{ in } kPa) + 0.00237(octane \text{ number})$$

<b>Item</b>	<b>Price</b>
Coal	\$33/metric ton delivered
Power	\$0.05/kWh
Peaking Power	\$0.10/kWh
Slag	\$5.5/metric ton
Sulfur	\$300/metric ton
Coal Tar/Liquid*	\$99.1/metric ton
Hydrogen <sup>†</sup>	\$35.3/1000 std m <sup>3</sup> (Case 3A)
	\$20.6/1000 std m <sup>3</sup> (Case 3B)
Natural Gas <sup>†</sup>	\$106/1000 std m <sup>3</sup> (Case 3A)
	\$61.8/1000 std m <sup>3</sup> (Case 3B)

\*Based on its fuel value at \$3/MM BTU  
<sup>†</sup> Case 3A prices are for West Virginia  
Case 3B prices are for Gulf Coast

**Table 4.3**  
**Estimated Value of Alcohol Fuel Additives**

Component	Blending Value (\$/liter)	Blending Value (\$/gal)
methanol	0.148	0.561
ethanol	0.235	0.893
n-propanol	0.185	0.699
n-butanol	0.183	0.693
n-pentanol	0.180	0.681
mixed alcohol product*	0.197	0.747
MTBE	0.223	0.845

\*value obtained based upon product distribution  
from alcohol synthesis reactor [7]

These values do not recognize the effects of substitution on the MTBE price should a less expensive competitive product be placed on the oxygenate market. The lowest price for which MTBE could be sold has not been determined. 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.

### 9.2.2 Measures of Economic Feasibility

The alcohol production process has been divided into two stages. The first stage entails those steps required to produce synthesis gas, while the second stage deals with the steps involved with the transformation of the synthesis gas into the alcohol fuel and waste. Since the alcohol product can be manufactured from synthesis gas derived from either coal or natural gas, the price of the synthesis gas derived from its respective source becomes a critical factor in determining the choice of feed stock. Thus, the prices for the respective syngases must be derived because they are intermediate products that are not marketed. Consequently, price data do not exist.

The manufacturing cost is defined as the sum of the raw materials and operating costs plus a capital recovery annuity, minus by-product credits. This model simply amortizes the installed capital investment over the anticipated life of the plant (which in this case is assumed to be twenty years) at a given interest rate (which we have assumed to be 10%, given current economic conditions). Besides utilities, the operating costs also include maintenance, insurance, plant overhead, and sustaining capital charges. These latter costs are estimated to be 1.5 times the annualized capital investment [11] (which is approximately equivalent to 17.6 percent of the total installed capital [17]).

### **9.3 Screening of Alternatives**

Two screening mechanisms have been employed for the purpose of eliminating and ranking technologies. The first process entails the calculation of the manufacturing cost for the mixed alcohols produced by the various technologies. These costs (in 1992 dollars) are current, identifiable and are calculated to include all by-product credits. Therefore, the process with the lowest manufacturing cost represents the best technology. The second screening alternative that was considered was overall energy efficiency. This method was considered to ensure that the optimal technology was selected given the level of uncertainty of future costs and prices. The thermal efficiencies were calculated based upon the total energy input in relation to the total energy output. Energy flows were also analyzed to determine which process provided the best alcohol conversion. This was measured by analyzing the total energy input in relation to the total energy content (heats of combustion) of the various products produced. The results of these methods are given in Section 6 of this report.