Chapter 8

Approach and Rationale

Coal-derived transportation fuels can be generated by indirect liquefaction in which coal is first converted to syngas and the syngas is then upgraded to motor fuels. The commercial feasibility of this conversion method depends upon the net cost of the syngas, the cost of syngas conversion, and the value of the finished products relative to existing competing products, such as gasoline, ethanol, and MTBE. In addition, the relative environmental costs of producing and using these competing fuels must also be compared.

Our approach is to study a series of cases (with the goal of producing gasoline oxygenate additives from coal-derived syngas), each characterized by discrete process choices. For cases that show distinct advantages, we would proceed to more detailed process analysis and optimization. The objective functions used to discriminate between alternatives are manufacturing cost per unit of mixed alcohol product and overall energy efficiency. The economies of scale for the cases are studied relative to both technical and market constraints. We have made several process choices, which are described in this section. These methodologies are described in more detail in Section 4.

8.1 Target Blends

To provide a production goal for the designs, target products were identified. All fuels for light-duty gasoline vehicles must be certified by EPA. Two blends already certified (i.e., granted waivers) are the DuPont blend [3,4] and OCTAMIX™.[5] These blends contain <5% (vol) methanol and >2.5% (vol) higher alcohols (C_2-C_4 for DuPont, C_2-C_8 for OCTAMIX™) plus 40 mg/liter of a corrosion inhibitor necessitated because water is soluble enough in methanol to corrode automobile gasoline distribution systems. We chose these certified blends as standards for this study for two reasons. First, the anticipated product slate from our process should satisfy the requirements of these certified blends without major purification. Second, this approach is also a conservative strategy. As future environmental regulations are largely unpredictable, we chose not to design around a less restrictive standard that might prove to be unacceptable under future regulations. All products produced would meet existing regulations.

8.2 Choice of Cases

Given the goals of the economic evaluation, a number of technological cases must be designed and tested. Five concerns guide the choice of cases.

1. A comparison of the manufacturing cost of syngas from coal with that from natural gas is needed. Since natural gas is the current lowest-cost source for all

manufactured syngas, this case is used as a benchmark by which to measure all projects using coal gasification. Hybrid cases are also investigated in order to uncover possible synergies between the two raw materials available to produce syngas.

2. An investigation of by-product production in coal gasification is needed since this requirement presents a number of production and marketing constraints that seriously impact the net cost of syngas and the resultant transportation fuels. For example, processes that convert coal to syngas without by-products can be economical only if their costs are less than the net costs of processes that co-produce syngas and by-products. Also, the production of by-products can present serious marketing problems. Lastly, the social costs of coal must be considered when the net costs of syngas process alternatives are compared.

3. A comparison of alternative modern gasifier technologies is essential.

4. A case is considered in which the higher alcohol fuel additives are by-products of a power generation facility.

5. Economic models must recognize present environmental regulation and the possibility of future changes.

Seven cases are chosen to the test range of possible technological and economic configurations identified as being important. The seven cases are shown in Table 3.1.

Table 3.1
Summary of Designs

Case Number	Gasifier	H_2/CO adjustment
1	Texaco	steam reforming of natural gas
2	Lurgi	pressure swing adsorption to separate excess H_2
3A/3B†	None (natural gas reformation only)	pressure swing adsorption to separate excess H_2
4	Texaco	sour gas shift converter
5	Shell	sour gas shift converter
6	Shell	steam reforming of natural gas
7‡	Texaco	sour gas shift converter

†The difference between these sub-cases is the price of natural gas.
‡In this case, higher-alcohols are a by-product of a power production facility.

They represent a broad range of cases, the details of which are given in Section 5 and in the Appendices. Our overall approach to these cases is that the alcohol synthesis and separation portion of the flowsheet is decoupled from the syngas production portion. This scheme is shown in Figure 3.1. Thus, the characteristic features of the various cases are their gasifier design and method for H_2/CO adjustment. For each case, the design downstream of the syngas cleaning is identical.

The natural gas case (Case 3) and IGCC case (Case 7) are chosen as a benchmarks. Although the goal of the study was to identify opportunities using coal-derived synthesis gas, such syngas is presently (for all gasifier types) more expensive than syngas produced from natural gas. Thus, Cases 3 and 7 present frames of reference for all case analyses. The Lurgi gasifier case (Case 2) was also chosen as a point of reference. This gasifier technology is proven, yet not state-of-the-art. This case allowed us to study the potential of producing additional by-products, as well as to quantify the improvements obtained by advances in gasifier design. The other five cases involve modern gasifiers (Texaco and Shell), each with H_2/CO adjustment by either water-gas shift or natural gas reformation. The slurry-fed Texaco design was chosen because it is a proven technology with many commercial installations. The Shell gasifier, with gas-conveyed feed, is representative of newer designs that are only now being built on a commercial scale.

8.3 Energy Park

The range of cases allowed us to use a holistic approach, which we call the *Energy Park* concept. 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. This means that all types of fuels, including coal and natural gas, should be considered as inputs. In fact, hybrid cases, such as Cases 1 and 6, were investigated to study potential synergies between raw materials. 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.

If energy is used more efficiently, not only are costs lowered, but pollution is also reduced. For example, a conventional steam-electric generation plant converts only 35 percent of the energy from combustion to usable electric energy. For the quantity of power produced, a proportional amount of pollutants is also produced. If the energy in the waste heat is captured, the overall efficiency can be improved. This increase in efficiency results in a decline in pollution per usable energy unit output. Thus, energy efficiency as well as costs can be used to determine the feasibility of a process. Therefore, more usable energy is obtained from the same amount of fuel.

Figure 3.1: Alternative Syngas and Alcohol Production Pathways