Chapter 10

Description of Cases

10.1 Process Concept

A generic process for converting coal to syngas to higher alcohol fuel additives is outlined in Figure 5.1. The oxygen plant provides oxygen for the gasifier. The sour gas shift converter adjusts the H₂/CO ratio to the desired ratio of 1.1/1 using the water gas shift reaction, with the necessary steam provided by vaporization of water used to slurry the coal. An alternative process might employ steam reforming of natural gas (CH₄ + H₂O \leftrightarrow CO + 3H₂) to adjust this ratio. Acid gas treatment and sulfur removal precede alcohol synthesis. The alcohol synthesis reactor is a shell-and-tube design with the MoS₂ catalyst in the shell. Use of the MoS₂ catalyst yields a product that is primarily C₁-C₅ linear alcohols [7]. Table 5.1 gives a typical reactor yield.

Table 5.1Typical Product Yields from MoS2 Catalyst based on40% CO Conversion	
carbon dioxide	32.00% (mol)
methane	9.45%
ethane	0.75%
methanol	13.46%
ethanol	28.08%
propanols	9.32%
butanols	3.13%
C ₅ alcohols	1.63%
methyl acetate	1.16%
ethyl acetate	1.02%
total	100%

10.2 Designs

The features of the seven cases were shown in Table 3.1. Detailed descriptions of each case (with flowsheet and flow tables) are included in the appendices. A very brief overview of each case is given below.

Case 1 is shown in the Appendix A, Figure A.1. The Texaco gasifier is oxygen blown, operates at high temperature (1300°C (~2400°F), 8 MPa (80 atm)), and is fed a coal-water slurry. This down-flow entrained design is currently being used in over 90

commercial applications world-wide. For larger scales we assume multiple trains. To enhance the H_2/CO ratio, natural gas is steam reformed.



Case 2 (Appendix B, Figure B.1) incorporates a Lurgi (dry-bottom) gasifier design. This gasifier is oxygen blown and operates at moderate temperatures (400°C (750°F), 2.8 MPa (28 atm)). It is the design used at the Great Plains Gasification Plant [11] and produces phenolic and related by-products. To reduce the H_2 /CO ratio, pressure swing adsorption is used to separate the excess H_2 .

Cases 3A and 3B (Appendix C, Figure C.1) are benchmark cases with natural gas as the feed. Through steam reformation, a syngas that is too rich in H_2 is produced. Pressure swing adsorption is used to separate the excess hydrogen. Some of the excess hydrogen is used to balance process power needs, and the remaining hydrogen is given a

value based on its heating value relative to that of natural gas (Table 4.2). The difference between Cases 3A and 3B are that the former uses a West Virginia natural gas price (106/1000 std m³, $3.00/10^{6}$ BTU) and the latter uses a Gulf Coast natural gas price (1.8/1000 std m³, $1.75/10^{6}$ BTU).

Case 4 is shown in the Appendix D, Figure D.1. As in Case 1, a Texaco gasifier is used. However, the hydrogen deficit is corrected by producing more syngas from the coal and then using a water-gas shift reactor to produce more hydrogen. Thus, more gasifiers are required in Case 4 than in Case 1.

Case 5 (Appendix E, Figure E.1) incorporates a Shell gasifier. As with the Texaco design, this gasifier is oxygen blown. It operates at high temperature and moderate pressure (1300°C (~2400°F), 2.8 MPa (28 atm)). However, the pulverized coal is conveyed to the gasifier in a gas stream (CO₂ in this case). This down-flow entrained design is not in current commercial use for coal gasification. However, it has been proven on pilot scale, and an integrated, combined-cycle, coal gasification power plant using this technology is under construction in The Netherlands [18]. For larger scales we assume multiple trains. To enhance the H₂/CO ratio, more syngas is produced from coal and a water-gas shift reactor is used.

Case 6 is shown in the Appendix F, Figure F.1. As in Case 5, a Shell gasifier is used. However, the hydrogen deficit is corrected by steam reformation of natural gas. Thus, fewer gasifiers are required in Case 6 than in Case 5.

Case 7 is shown in the Appendix G, Figure G.1. It is an IGCC power plant with a net base load capacity of 500 MW and an additional 100 MW of peaking capacity (for 2 two-hour periods per day) derived from burning methanol separated from the mixed alcohol produced in the alcohol synthesis loop. Approximately 112 million liters/yr (30 million gallons/yr) of higher alcohols can be produced as a by-product of this process for use as oxygenates.

In all of the designs, the purge from the alcohol synthesis loop is used to generate power. Additionally, steam produced by recovering heat from the gasifier outlet is also used to generate power.