Chapter 13

Recommendations and Future Work

13.1 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.

13.2 Sensitivity Analysis

13.2.1 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.

13.2.2 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.

13.3 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.

13.4 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.

References for chapters 7-13

1. Wake, J., H. Schwendener and J. Shimosato, "Gasoline Octane Improvers" CEH Marketing Research Report, SRI International, Sept. 1990.

2. Gibson, T. and T. Sasano, "Plasticizer Alcohols (C_4-C_{13})" CEH Marketing Research Report, SRI International, Aug. 1990.

3. 51 FR 39800 [*Federal Register*, vol. 51, p. 39800 (1986)].

4. 52 FR 18736 [*Federal Register*, vol. 52, p. 18736 (1987)].

5. 53 FR 43768 [*Federal Register*, vol. 53, p. 43768 (1988)].

6. "Houston Area Medium-BTU Coal Gasification Project, Feasibility Study -- Final Report, Volumes 1-3," DOE Contract #DE-FGO1-80-RA-50382, prepared by the Linde Division of Union Carbide Corporation, June 1982.

7. Nirula, S., "Dow/Union Carbide Process for Mixed Alcohols from Syngas," PEP Review # 85-1-4, Process Economics Program, SRI International, March 1986.

8. Pavone, A., "Options for Procuring Oxygen," PEP Review #89-3-3, Process Economics Program, SRI International, January 1991.

9. "Methane Emissions From Coal Mining: Issues and Opportunities For Reduction," U.S. Environmental Protection Agency, EPA/400/90/008, prepared by ICF Resources Incorporated, September 1990.

10. "Coal Data," National Coal Association, Washington, DC, 1993.

11. Dingler, J. E., S. Nirula and W. Sedriks, "Costs of Synthesis Gases and Methanol," SRI report #148, Process Economics Program, SRI International, February 1983.

12. "Process Descriptions, Baseline Design/Economics for Advanced Fisher-Tropsch Technology," Fourth Progress Meeting, DOE Contract #DE-AC22-91PC90027, prepared by Bechtel Corporation, San Francisco, CA, March 1993.

13. "Coal Gasification Systems: A Guide to Status, Applications and Economics," EPRI Report AP-3109, Final Report, June 1983.

14. Rock, K. L., T. de Cardenas and L. Fornoff, "The New Refinery Challenge," *Fuel Reformulation*, Nov/Dec, 1992, p. 42.

15. "Annual Energy Review 1993," DOE/EIA-0384(93), p.181, July 1994

16. Dale, Charles, EIA, Personal Communication.

17. Peters, M. S. and K. D. Timmerhaus, *Plant Design and Economics for Chemical Engineers (4th ed.)*, McGraw-Hill, New York, 1991, pp. 210-211.

18. Bayens, C. A. and G. A. Cremer, "Update on Projects using Shell Coal Gasification Process," *Proceedings of the Tenth Annual International Pittsburgh Coal Conference*, Pittsburgh, PA, September, 1993, pp. 366-371.

19. Fleisch, Theo H., Plenary Presentation, DOE Coal Liquefaction and Gas Conversion Contractors Review Conference, Pittsburgh, PA, August 29, 1995.

20. "Annual Energy Outlook 1992," DOE/EIA-0383(92).

21. "Federal Reserve Bulletin," No.79, Jan 1993.

22. Whiting, W. B., T.-M. Tong and M. E. Reed, "Effect of Uncertainties in Thermodynamic Data and Model Parameters on Calculated Process Performance," *Ind Eng Chem Res*, **32**, 1367 (1993).

23. Brown, D. M., Air Products and Chemicals, personal communication.