ChE 183
Major 3

Styrene Production

Styrene demand is expected to increase in the near future. Therefore, we are considering construction of a grass-roots facility to increase our styrene capacity. Therefore, your assignment is to complete a preliminary design of a 100,000 tonne/y styrene production facility, which will operate for an 8000 hour year. Additionally, a new catalyst has been developed with kinetics that enhances the selectivity for styrene. We would like you to do a preliminary evaluation of the profitability of such a grass-roots facility.

Styrene Production Reaction Kinetics

The reactions for styrene production for our new catalyst are as follows:

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \underset{2}{\overset{1}{\rightleftarrows}} \underset{\text{styrene}}{C_6H_5C_2H_3} + \underset{\text{hydrogen}}{H_2} \tag{1}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{3}{\longrightarrow} \underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \tag{2}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{hydrogen}}{H_2} \overset{4}{\longrightarrow} \underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{methane}}{CH_4} \tag{3}$$

Kinetics (subscripts on r refer to reactions in Equation (1) – (3):

$$r_1 = 8.44\times10^9 \exp\left(-\frac{35500}{RT}\right)p_{eb} \tag{4}$$

$$r_2 = 1503\exp\left(-\frac{5988}{RT}\right)p_{sty}\,p_{hyd} \tag{5}$$

$$r_3 = 7.21\times10^9 \exp\left(-\frac{57500}{RT}\right)p_{eb} \tag{6}$$

$$r_4 = 2.09\times10^6 \exp\left(-\frac{43500}{RT}\right)p_{eb}\,p_{hyd} \tag{7}$$

where p is in kPa, T is in K, R = 1.987 cal/mol K, and r_i is in mol/m^3 reactor s.

Assignment

Specifically, you are to prepare the following by 9:00 am, Monday, February 21, 2000:

1. a recommended optimum design for the grass-roots facility
2. a neatly drawn and labeled PFD for the grass-roots facility
3. a profitability analysis for the grass-roots facility
4. a written report, conforming to the guidelines, detailing the information in items 1 through 3, above
5. a legible, organized set of calculations justifying your recommendations, including any assumptions made
6. a signed copy of the attached confidentiality statement.

Other Information

The objective function should be the net present value (NPV). Assume that the capital cost is paid in two installments prior to plant start-up, and that working capital is 20% of the fixed capital investment. Plant life is considered to be 10 years. The internal hurdle rate is 10%, after taxes. MACRS depreciation should be used. Prices for ethylbenzene listed in *Chemical Market Reporter* may be artificially inflated because most ethylbenzene manufactured is used in the same plant to make styrene. If this causes the process to be unprofitable, your new objective function should be the break-even price for ethylbenzene using the economic parameters above.

Based on the location of this plant, excess steam cannot be sold for credit.

For flash tank sizing and for heat transfer coefficients, use the heuristics in Chapter 9 of your text[1]. For distillation columns, use the heuristics only for determining a proper height to diameter ratio. Do the rest of the design yourself.

For a packed bed reactor without heat transfer, cost it at a value of three times the cost of a vessel. For a shell and tube packed bed with heat transfer, if a heat transfer fluid loop is used or if steam is condensed in the shell, cost the reactor as a heat exchanger and multiply the cost by a factor of 5.

The three-phase flash can be simulated using the regular flash unit with three exit streams. All that is required is that you specify two outlet conditions. Since there is no heat transfer in this device, you should use the mode where the outlet temperature and pressure are identical to the inlet values. Any light gases not entering the top stream may be assumed to be vented from the reflux drum of the first tower and mixed with the hydrogen/light-gas stream prior to compression. This may be simulated with a component separator prior to the first tower, but the actual PFD should show the vent on the reflux drum.

It should be assumed that the minimum pressure required for all streams leaving the process to reach their destination is 2 bar.

Report Format

This report should conform to the guidelines. It should be bound in a folder that is not oversized relative to the number of pages in the report. It should be organized like a standard design report. Figures and tables should be included as appropriate. An appendix should be attached that includes sample calculations and a Chemcad report, for the optimum case, that does not contain stream properties. The appendix should be easy to follow. The confidentiality statement should be the very last page of the report.

The written report is a very important part of the assignment. Poorly written and/or organized written reports may require re-writing. Be sure to follow the format outlined in the guidelines for written reports. Failure to follow the prescribed format may be grounds for a re-write.

Oral Presentation

You will be expected to present and defend your results some time between February 23 and February 28, 2000. Your presentation should be 15-20 minutes, followed by about a 30 minute question and answer period. Make certain that you prepare for this presentation since it is an important part of your assignment. You should bring at least one hard copy of your slides to the presentation, and should be handed out at the beginning of the presentation.

Late Reports

Late reports are unacceptable. The following severe penalties will apply:

- late report on due date before noon: one letter grade (10 points)
- late report after noon on due date: two letter grades (20 points)
- late report one day late: three letter grades (30 points)
- each additional day late: 10 additional points per day

References

1. Turton, R., R. C. Bailie, W. B. Whiting and J. A. Shaeiwitz, *Analysis, Synthesis, and Design of Chemical Processes*, Prentice Hall, Upper Saddle River, NJ, 1998.

Appendix
Other Pertinent Information

Reaction Equilibrium

Styrene reaction may be equilibrium limited

$$K = \left(\frac{y_{sty} y_{hyd} P}{y_{eb}} \right)$$

$$\ln K = 15.5408 - \frac{14852.6}{T}$$

where T is in K and P is in bar.

Equilibrium calculation:

$$C_6H_5C_2H_5 \underset{2}{\overset{1}{\rightleftarrows}} C_6H_5C_2H_3 + H_2$$

$$\begin{array}{ccc} 1 & 0 & 0 \\ 1-x & x & x \end{array}$$

$\text{total} = N + 1 + x$ includes N moles of inerts/moles ethylbenzene

$$K = \frac{x^2 P}{(1-x)(N+1+x)}$$

where P is in bar.