ChE 456
Spring 2011
Major 2

Styrene Production

Background

Your company has been requested to complete a new design of a styrene process, produced from ethylbenzene. The new plant capacity is 80,000 tonne/y, with an 8350-hour year.

Assignment

Your assignment is to provide a comprehensive process design for this new plant. Specifically, you are to prepare the following by 9:00 a.m., Monday, February 21, 2011:

1. Prepare a written report detailing your optimized process design for the new process subject to the constraints provided. The report should:

   - include a PFD that shows all the major equipment and process and utility streams. This PFD should be drawn using the standard icons in CorelDraw and should be legible, uncluttered, with all major equipment numbered, and all process streams identified by number. The PFD should be drawn in landscape format. Major control loops should also be drawn on the diagram.
   - include a flow table corresponding to the PFD requested above.
   - include a table with the design details (height, length, area, number of trays, power, etc.) of all major equipment needed for the process.
   - include the utility requirements for all equipment. Results for utility costs should be presented either as a table or in a figure, but not both.
   - include the cost of manufacture for the process. Results for cost of manufacture should be presented either as a table or in a figure, but not both.
   - include the capital costs (grass roots) for all equipment. Results for capital costs should be presented either as a table or in a figure, but not both.
   - include an analysis of the economics for the project, using a basis of a 2-year construction period (60% first year, and 40% second year – land is already owned), a 10% after-tax rate of return, a 10-year operating life, and a taxation rate of 45%. The objective function is the break-even price of ethylbenzene, since ethylbenzene is produced on site, and published “spot” prices are inflated.
   - include a list of raw material costs for the plant.

2. An appendix should be included with its own table of contents. Page numbering may continue from the end of the report or it may restart. This appendix should include:

   a. a converged Chemcad report for your proposed design should be included in the Appendix, using the consolidated report option. Do not include a full list of stream properties, but do include stream flows (mass and moles), unit operations, convergence results, and any other data relevant to your design. You should also include a copy of the Chemcad flowsheet for the proposed design.

   b. Excel spreadsheets for all capital cost estimations (using CACPCOST) and the cash flow diagrams.

   c. a legible, organized set of calculations justifying your recommendations, including any assumptions made. The appendices should have an accurate table of contents to allow the reader to find any particular calculation quickly.

Deliverables

Specifically, you are to deliver the following by 9:00 a.m., Monday, February 21, 2011:

1. Prepare a written report, conforming to the guidelines, detailing the information in items 1 and 2, above.
2. Attach a signed copy of the attached confidentiality statement.

Report Format

The written report is a very important part of the assignment. Reports that do not conform to the guidelines will receive severe deductions and will have to be rewritten to receive credit. Poorly written and/or organized written reports may also require rewriting. Be sure to follow the format outlined in the guidelines for written reports.

Oral Presentation

You will be expected to present and defend your results some time between February 21, 2011, and February 25, 2011. 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 two hard copies of your slides to the presentation and to hand out before beginning the presentation.

Other Rules

You may not discuss this major with anyone other than the instructors (or your partner). Discussion, collaboration, or any other interaction with anyone other than the instructors or your partner is prohibited. Violators will be subject to the penalties and procedures outlined in the University Procedures for Handling Academic Dishonesty Cases (see p. 45 of 2009-11

Undergraduate Catalog (http://coursecatalog.wvu.edu/fullcatalogs/09-11catalog.pdf) or follow the link http://www.arc.wvu.edu/rightsa.html).

Consulting is available from the instructor. Chemcad consulting, *i.e.*, questions on how to use Chemcad, not how to interpret results, is unlimited and free, but only from the instructors. Each individual (team) may receive five free minutes of consulting from the instructors. After five minutes of consulting, the rate is 2.5 points deducted for 15 minutes or any fraction of 15 minutes, on a cumulative basis. The initial 15-minute period includes the 5 minutes of free consulting.

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

Appendix 1
Design Criteria for Unit 400

- Feed
  - available from another part of plant at 135°C and 200 kPa
  - composition
    - 97 mol% ethylbenzene
    - 2 mol % toluene
    - 1 mol % of benzene
- Design basis = 80,000 tonne/yr of pure styrene – this should be contained in the product stream – with a styrene content >99.8 wt% as a liquid at 200 kPa
- Chemical costs may be obtained from http://www.icis.com/StaticPages/a-e.htm.
- The cost for the initial charge of catalyst is negligible.
- The catalyst maximum temperature is 600°C.
- Value of superheated steam = $8/GJ (above saturation) if returned to steam plant
- Suggested optimizations include, but are not limited to
  - type of steam used
  - reactor configuration (adiabatic, staged adiabatic with interheating, reactor with heating, hot shot interstage feed, etc.)
  - separation sequencing
  - parametric optimization of most significant parameters
- The reactors must be priced as user-added entries to Capcost, or substitute equipment must be used. For an adiabatic, packed bed reactor, use the cost of a vessel of appropriate size. The *L/D* ratio should be no less than five. For a shell-and-tube reactor, use twice the cost of a heat exchanger with the appropriate heat-transfer area.

Appendix 2
Reaction Kinetics and Equilibrium

The reactions for styrene production are as follows:

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \underset{k_2}{\overset{k_1}{\rightleftarrows}} \underset{\text{styrene}}{C_6H_5C_2H_3} + \underset{\text{hydrogen}}{H_2} \tag{1}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{k_3}{\longrightarrow} \underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \tag{2}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{hydrogen}}{H_2} \overset{k_4}{\longrightarrow} \underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{methane}}{CH_4} \tag{3}$$

Kinetics (subscripts on r refer to reactions in Equation (1) – (3) (adapted from Snyder, J. D. and B. Subramaniam, *Chem. Engr. Sci.*, **49**, 5585-5601 (1994) – the positive activation energy can arise from non-elementary kinetics and/or from reversible reactions:

$$r_1 = 1.177 \times 10^8 \exp\left(-\frac{21{,}708}{RT}\right) p_{eb} \tag{4}$$

$$r_2 = 20.965 \exp\left(\frac{7804}{RT}\right) p_{sty}\, p_{hyd} \tag{5}$$

$$r_3 = 7.206 \times 10^{11} \exp\left(-\frac{49{,}675}{RT}\right) p_{eb} \tag{6}$$

$$r_4 = 1.724 \times 10^6 \exp\left(-\frac{21{,}857}{RT}\right) p_{eb}\, p_{hyd} \tag{7}$$

where p is in bar, T is in K, R = 1.987 cal/mol K, and r_i is in mol/m^3 reactor s. When simulating this, or any reactor in Chemcad, the units for the reactor may be set separately from the units for the rest of the simulation in the “more specifications” tab. The reaction units in Chemcad must be moles/reactor volume/time.

The styrene reaction may be equilibrium limited, and the equilibrium constant is

$$K = \left(\frac{y_{sty} y_{hyd} P}{y_{eb}} \right) \tag{8}$$

and

$$\ln K = 15.5408 - \frac{14{,}852.6}{T} \tag{9}$$

where T is in K and P is in bar.

other data:

bulk catalyst density = 1282 kg/m^3
void fraction = 0.4