ChE 456
Spring 2008
Major 2

Production of Ethanol via the Vapor-Phase Hydration of Ethylene

Background

Plans to implement the original design of this facility have been shelved in part due to a new business opportunity that has arisen. Specifically, a new source of lower-grade, but relatively inexpensive, ethylene has been found. Our client (Seastraight Chemicals, Corp.) is negotiating a contract for long-term purchases of this ethylene stream and want to be ready with a technically correct and economically optimized process by the end of February, 2008. To this end, they have contracted us to provide a design for a 40,000 tonne/yr plant to convert ethylene to ethanol. The stream factor for this new plant is 0.975, and the specifications of the feed, ethanol product, and utilities are given in an appendix to this document.

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 25, 2008:

1. Prepare a written report detailing your optimized process design for the new plant under the constraints given for this process. 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 a table with the utility requirements for all equipment.

   - include a cumulative, discounted, after-tax, cash-flow diagram for the project, using a basis of a 2-year construction period, an 8% after-tax rate of return, and a 10-year operating life. Assume a taxation rate of 45%.

   - include a list of raw material costs for the plant.

2. Include a converged Chemcad report for your proposed design. Do not include a full list of stream properties, but do include stream flows, unit operations, convergence results, and any other data relevant to your design. This report should be presented as an appendix.

3. Include, as an appendix, Excel spreadsheets for all capital cost estimations (using CACPCOST) and the cash flow diagrams.

4. Include, as an appendix, 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 quickly any particular calculation.

Deliverables

Specifically, you are to prepare the following by 9:00 a.m., Monday, February 25, 2008:

1. Prepare a written report, conforming to the guidelines, detailing the information in items 1 - 4, 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 25, 2008, and March 5, 2008. 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 hand it out before beginning the presentation.

Other Rules

You may not discuss this major with anyone other than the instructors. Discussion, collaboration, or any other interaction with anyone other than the instructors is prohibited. Violators will be subject to the penalties and procedures outlined in the University Procedures for Handling Academic Dishonesty Cases (see p. 48 of 2007-09 Undergraduate Catalog or follow the link http://www.arc.wvu.edu/rightsa.html).

Consulting is available from the instructors. 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 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 200

- Feed ethylene specifications
    - available from pipeline at a pressure of 5,000 kPa and ambient temperature
    - composition
        - ≤ 5 ppm acetylene
        - ≤ 4.5 mole % of ethane
        - ≤ 0.5 mole % of methane
        - balance is ethylene
- Design basis = 40,000 tonne/yr of pure ethanol – this should be contained in a crude ethanol stream with an ethanol content >94 wt% at a pressure of 200 kPa and as a saturated liquid.
- Final purification and dehydration of ethanol will be performed by client
- Stream Factor = 0.975
- Cooling water is available at 30°C and 5 bar, should be returned at 40°C for design conditions, and never should the return temperature exceed 45°C. The cost of cooling water is $0.354/GJ.
- Fuel gas should be used for all fired heaters (assume natural gas content = 100% methane) at a cost of $10/GJ (based on lower heating value).
- Steam available for process heating:
    - High pressure – saturated at 42 bar available at a cost of $9.83/GJ
    - Medium pressure – saturated at 11 bar available at a cost of $8.22/GJ
    - Low pressure – saturated at 6 bar available at a cost of $7.78/GJ
- Wastewater, at a temperature ≤ 40°C and containing organics with a total concentration of less than 5000 ppm, is sent to a centralized treatment facility at a cost of $100/1000m^3.
- Selling price for ethanol is $2.90/gal
- Cost of ethylene is $0.29/lb

Appendix 2 – Information on Reaction Kinetics (same as in previous assignment)

Most ethanol (approximately 85%) manufactured in the U.S. comes from some form of fermentation process. However, a small amount is manufactured via the catalytic, gas-phase hydration of ethylene. The main reaction is

$$\underset{ethylene}{C_2H_4 + H_2O} \underset{r_2}{\overset{r_1}{\longleftrightarrow}} \underset{ethanol}{C_2H_5OH} \tag{1}$$

Where r_1 and r_2 are the forward and reverse rates, respectively. Experimental analysis of the performance of this catalyst [1], gives the following expressions for these reaction rates:

$$r_1 = \frac{k_1 p_W p_E}{\left(1 + K_W p_W + K_E p_E + \cancel{K_A p_A}\right)^2} \tag{2}$$

and

$$r_2 = \frac{k_2 p_A}{\left(1 + K_W p_W + K_E p_E + \cancel{K_A p_A}\right)^2} \tag{3}$$

where

$$k_1[\text{kmol/m}^3\text{cat/h/atm}^2] = 1.7723 \times 10^{-9} \exp\left(\frac{91{,}130}{RT[\text{K}]}\right)$$

$$k_2[\text{kmol/m}^3\text{cat/h/atm}] = 1.3865 \times 10^{-2} \exp\left(\frac{43{,}915}{RT[\text{K}]}\right)$$

$$K_W[\text{atm}^{-1}] = 1.2328 \times 10^{-17} \exp\left(\frac{162{,}730}{RT[\text{K}]}\right)$$

$$K_E[\text{atm}^{-1}] = 2.0850 \times 10^{-4} \exp\left(\frac{35{,}368}{RT[\text{K}]}\right)$$

and the activation energy is given in kJ/kmol, and p_i is measured in atmospheres.

Under the conditions used in commercial reactors, the last term in the denominator is negligible and may be ignored. Also note that the exponential terms in the numerator and denominator are all positive. This is an artifact of the lumping together of reaction rate constants and adsorption equilibrium constants in Equations (2)-(3). However, the net effect of temperature on the overall forward and reverse reactions is that the overall rates increase with increasing temperature, which is consistent with Arrhenius-type behavior.

Along with the desired, forward, reaction shown in Equation (1), ethanol can also dehydrate to form diethyl ether as follows:

$$\underset{ethanol}{C_2H_5OH} \leftrightarrow H_2O + \underset{diethyl\ ether}{(CH_3CH_2)_2O} \tag{4}$$

The catalyst used in the process of interest is zirconium tungstate, and it effectively suppresses the diethyl ether reaction shown in Equation (4). It has a void fraction of 0.5.

In addition, any acetylene in the ethylene feed may be converted to acetaldehyde, which is tolerable in the final ethanol product at only very low concentrations (< 1ppm).

$$\underset{ethylene}{C_2H_2} + H_2O \xrightarrow{r_3} \underset{acetaldehyde}{CH_3CHO} \tag{5}$$

The rate for this reaction is given by:

$$r_3 = k_3[\text{kmol/m}^3\text{cat/h/atm}]\, p_{Acet}[\text{atm}] \tag{6}$$

where

$$k_3 = 1\times10^{-4}\exp\left[-\frac{25{,}000[\text{kJ/kmol}]}{\text{RT}[K]}\right] \tag{7}$$

Reference

1. Momose, H., Kusumoto, K., Izumi, Y., and Y. Mizutani, "Vapor-Phase Direct Hydration of Ethylene over Zirconium Tungstate Catalyst," *J. Catalysis*, **77**, 23-31 (1982).