ChE 456
Spring 2007
Major 2

Production of Formalin

Background

Your job is to prepare a preliminary design for the new 50,000 tonne/y formalin from methanol plant. The new plant will be integrated with a wood-products facility, so it will not be necessary to have a large storage tank at the end of the process, since, under normal conditions, the formalin will be fed directly to the resin production portion of the wood products facility. An emergency storage tank, with appropriate controls, sized for a three-day supply of formalin is suggested; but, under normal operating conditions, formalin product should not pass through this tank.

A new catalyst has been identified that will simplify the reactor design and operation. This is an oxide catalyst that has approximately uniform activity over a one-year period and catalyzes the oxidation reaction but not the disproportionation reaction:

$$CH_3OH + \tfrac{1}{2}O_2 \rightarrow HCHO + H_2O \qquad (1)$$

The appropriate reactor design is a key consideration. It is believed that that a shell-and-tube configuration with heat removal or staged adiabatic packed beds with intercooling would be two good initial choices. This reaction operates at "methanol lean" conditions, *i.e.*, below the LFL of methanol of 6 mole%. Typical operating conditions for maximum catalyst activity are 200°C to 350°C, and pressures just above atmospheric.

This plant will be constructed in an area subject to seasonal fluctuations in ambient temperature. As such, the temperature of available cooling water is expected to vary between 25°C and 35°C over the course of a year.

Assignment

Your assignment is to provide:

1. an optimized design of a plant to make formalin from methanol using the oxide catalyst

2. a clear operating policy for key pieces of equipment affected by the seasonal cooling water variation

3. an economic evaluation (after-tax DCFROR, marginal tax rate assumed to be 40%, 5-year MACRS) of the process, with a recommendation as to whether to construct the plant. Assume that the desired, after-tax rate of return is 9% over 10 years, with a two-year construction period. Capital costs are 60% at the end of year 1 and 40% at the end

of year 2. The land is already owned, there is no salvage value, and working capital is 50% of the first-year's operating costs (including raw materials).

Report Format

This report should be comprehensive and 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. Figures and tables should be included as appropriate. An appendix should be attached that includes items such as Chemcad output and sample calculations. These calculations 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. 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 re-writing. Be sure to follow the format outlined in the guidelines for written reports.

The following information, at a minimum, must appear in the main body of the final report:

1. a computer-generated PFD (not a Chemcad PFD) for the recommended optimum case,

2. a stream table containing the usual items,

3. a list of new equipment for the process, including bare module and installed costs, plus equipment specifications (presented with a reasonable number of significant figures),

4. a summary table of all utilities used,

5. a clear summary of alternatives considered and a discussion, supported with figures, of why the chosen alternative is superior,

6. a clear economic analysis which justifies the recommended case

7. a clear discussion of the operating policies for seasonal operation

8. a Chemcad report only for your optimized case (in the Appendix). This must contain the equipment connectivity thermodynamics, and overall material balance cover pages, stream flows, equipment summaries, tower profiles, and tray design specifications (if you use Chemcad to design the trays). It should not contain stream properties. Missing Chemcad output will not be requested; credit will be deducted as if the information is missing.

Oral Presentation

You will be expected to present and defend your results some time between February 19, 2007 and February 23, 2007. 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 (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
Reaction Kinetics

The reaction engineering group has obtained the following kinetic information on the methanol oxidation reaction.

$$CH_3OH + \tfrac{1}{2}O_2 \rightarrow HCHO + H_2O \tag{2}$$

The rate expression is

$$-r_m\,[mole\,/\,g\ catalyst\ \ hr] = \frac{k_1 p_m}{1 + k_2 p_m} \tag{3}$$

where p is a partial pressure in atm, and m refers to methanol. The rate expression in Eq. (2) is only valid when oxygen is present in excess. The catalyst bulk density is 1500 kg catalyst/m^3 of reactor volume. The constants in Eq. (2) are defined as

$$\ln k_1 = 12.50 - \frac{8774}{T} \tag{4}$$

$$\ln k_2 = -17.29 + \frac{7439}{T} \tag{5}$$

where T is in Kelvin.

Appendix 2
Chemcad Hints

Solutions of formaldehyde and water are very non-ideal. Individually, the volatilities are, from most volatile to least volatile, formaldehyde, methanol, water. However, formaldehyde associates with water so that when this three-component mixture is distilled, methanol is the light key and water is the heavy key. The formaldehyde will "follow" the water. The ESDK *K*-value package in Chemcad simulates this appropriately. Latent heat should be used for enthalpy calculations. The expert system will recommend these choices.

When simulating an entire process, we recommend using the shortcut distillation column, within the process for the methanol-water/formaldehyde distillation. SCDS or TOWR should then be used as a separate item to simulate the column based on the results obtained from the shortcut column.

For the reactor, you must set the local units within the kinetic reactor calculation to correspond to the units of the chemical reaction. Remember that Chemcad only accepts rate data on a per volume of reactor basis. You may choose any activation energy unit. Then, you must multiply the numerator of the second term in Equations 4 and 5 by that value, since the reaction expression for Chemcad assumes the form $\exp[-E/RT]$.

Since the reactor effluent to be purified will have non-condensable gases, some of them will partition into the liquid phase in any initial separation. If these are included in a distillation column feed, the simulation algorithm in Chemcad will try to condense them, and the top temperature may appear inappropriately low. Therefore, to avoid this situation, a component separator should be placed in the simulation just before the distillation column to remove all of the non-condensable gases. In the simulation, this stream should be mixed with the off-gas stream. However, in the actual process, these gases would be removed from a "partial-total" condenser at the top of the distillation column. The non-condensable gases are vented off (the "partial" component), while all components involved in the separation are condensed completely (the "total" component). This should be appropriately illustrated on your PFD, with the non-condensable gases mixing with the off-gas stream.

Appendix 3
Other Information

1. Assume 1500 W/m^{2}K for the Dowtherm or molten salt. Assume the reaction-side heat transfer coefficient is 60 W/m^{2}K.

2. To size a flash vessel, take the liquid flowrate (vol/time) and assume a 10 min residence time. This gives a volume. Then double this value to get the vessel volume. To determine the L/D ratio in the flash vessel, assume a vapor flowrate of 1 m/s and determine the cross sectional area. This gives the diameter. The height (L) is then obtained from the volume.

3. The catalyst diameter is 5 mm, and its porosity is 0.4.

4. To determine the cost of a reactor, for a shell-and-tube reactor cost = 2(Cost the heat exchanger based on area + cost of vessel), and for an adiabatic reactor, cost = 2(cost of vessel).