ChE 456
Spring 2003
Major 2

Drying Oil Production

Drying oils are additives to paints and varnishes to aid in the drying process when these products are applied to surfaces. It has been determined that the market for drying oil in Southeast Asia is expanding. Therefore, we are planning to construct a new facility to increase capacity in that region. Specifically, you are to design a new facility that produces 25,000 tonne/y of 99 wt % drying oil. The by-product acetic acid may be sold at a purity of 99.5 wt %. The facility is to manufacture drying oil (DO) from acetylated castor oil (ACO). Both of these compounds are mixtures. However, for simulation purposes, acetylated castor oil is modeled as palmitic (hexadecanoic) acid ($C_{15}H_{31}COOH$) and drying oil is modeled as 1-tetradecene ($C_{14}H_{28}$). In an undesired side reaction, a gum can be formed, which is modeled as 1-octacosene ($C_{28}H_{56}$).

Constraints

There are two constraints to this new design that are different from operations at our Northern Pennsylvania facility. First of all, the only use for steam is within the drying oil process; there is no credit available for any steam produced in excess of this amount. Secondly, the technical services division has determined that the temperature of any stream containing ACO or DO downstream of the filter must be maintained below 300°C to avoid fouling due to gum formation.

Reaction Kinetics

The reactions and reaction kinetics are as follows:

$$\underset{\text{ACO}}{C_{15}H_{31}COOH(l)} \xrightarrow{k_1} \underset{\text{acetic acid}}{CH_3COOH(g)} + \underset{\text{DO}}{C_{14}H_{28}(l)} \tag{1}$$

$$\underset{\text{DO}}{2C_{14}H_{28}(l)} \xrightarrow{k_2} \underset{\text{gum}}{C_{28}H_{56}(s)} \tag{2}$$

where

$$-r_1 = k_1 C_{ACO} \tag{3}$$

$$-r_2 = k_2 C_{DO}^2 \tag{4}$$

and

$$k_1 = 5.538 \times 10^{13} \exp(-44{,}500 / RT) \tag{5}$$

$$k_2 = 1.55 \times 10^{26} \exp(-88{,}000 / RT) \tag{6}$$

The units of reaction rate, r_i, are kmol/m^{3}s, and the activation energy is in cal/mol (which is equivalent to kcal/kmol).

Separators

The gum filter should be simulated as a perfect separator. It should be shown on the PFD as it was shown on the first major. The capital cost of the vessel and filter is given by:

$$\text{Filter Cost} = \$150{,}000 \left[\frac{\text{Mass Flow of Reactor Effluent(kg/h)}}{10{,}700} \right]^{0.6}$$

The material flowing through the filter must be liquid. The operating cost is shown below.

You must choose the operating pressures for each column subject to constraints of operating temperature and available utilities. If Dowtherm A is to be used, it should be remembered that its maximum operating temperature is 400°C. If vacuum columns are needed, pressure drop becomes a significant concern. As an alternative to tray towers, packed towers with a low-pressure-drop structured packing may be used. The cost of these is available in Capcost. The packing factor as defined in Wankat[1], p. 424, is that for Koch Flexipac #2. Assume the HETP for the structured packing to be 1.5 m (see the definition of HETP in Wankat[1], p. 418), and that the pressure drop is 0.2 kPa/m.

Reactors

You should consider both an adiabatic and an isothermal reactor. Since the reaction is endothermic, a heat source will have to be provided for an isothermal reactor. The temperature and pressure of the reactor are suggested decision variables.

Heat Exchangers

When designing heat exchangers, you should make sure that the number of shell- and tube-passes are specified for exchangers in which no phase change occurs for either fluid. For reboilers, you should not exceed a maximum heat flux of 25 kW/m^2. This may require the throttling and desuperheating of steam utilities in order to reduce the temperature driving force in the reboilers so as not to exceed this maximum flux.

Economics

For this new process, the measure of profitability should be the NPV. You should use a 10%, after-tax rate of return, 5-year MACRS depreciation, a 25% tax rate, and a 10-year lifetime. Construction is estimated to take two years, with 60% of the capital investment at the end of the first year and 40% at the end of the second year. The cost of land is $8 million, and the working capital needed is 50% of the raw material cost in the first year. The fixed capital investment of the plant (FCI_L) should be estimated using the grass-roots cost from the CAPCOST program that is installed on the computers in the undergraduate room.

The values of the raw material and products are as follows:

ACO – $0.59/kg

Acetic acid – $0.99/kg

DO – $1.19/kg

Gum – has no value, operating cost for the filter and disposal cost for the gum are:

$$\text{cost of gum filtration and disposal (units of \$/kg DO leaving reactor)} = 10^{-3}[(\text{ppm gum leaving reactor}) - 1]$$

Deliverables

Specifically, you are to prepare the following by 9:00 a.m., Monday, February 24, 2003:

1. an optimized, grass-roots design for the new drying oil facility,
2. a written report, conforming to the Department guidelines, detailing the design,
3. a legible, organized set of calculations justifying your recommended design, including any assumptions made,
4. a signed copy of the attached confidentiality statement.

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 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 24, 2003 and March 4, 2003. 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 (begins on p. 48 of 2001-03 Undergraduate Catalog).

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

References

1. Wankat, P., *Equilibrium Staged Separation Processes*, Prentice Hall, Upper Saddle River, NJ, 1988.

Appendix 1

Chemcad Hints

In order to simulate this process, it is necessary for you to add gum as a compound to the Chemcad databank. This has already been done in room 453, and the simulation used for the first major is also in the CC5data folder. However, if you save the job to a zip disk or floppy disk, it will not contain the new component. You must export the file rather than just saving or copying it for it to contain the new component information. Therefore, it may be beneficial for you to add this component to the databank on your home computer.

The procedure is as follows:

1. From the Thermophysical menu, click on databank and new component.

2. In the dialog box that is shown, enter a name for the compound (we used gum), the molecular weight (392) and the boiling point (431.6°C). Click on group contribution - Joback. This will use a group contribution method to estimate properties. Then, click OK.

3. In the next dialog box, you must put in the correct groups. There is 1 $-CH_3$ group, 25 $>CH_2$ groups, 1 $=CH_2$ group, and 1 $=CH-$ group. Then, click OK.

4. It will ask you if you want to save this component. Click yes. It will probably assign it as component number 8001.

5. If you want to check information or add more information, you can now go to Thermophysical, databank, view-edit. Then, type in the new component number. When the next menu list comes up, one thing you can do, for example, is add the chemical formula for gum or add the correct chemical name under synonyms. However, these are not necessary to run simulations using this new compound.

6. Be sure that the new compound, gum, is in your component list for the current job.

It is suggested that you simulate the process without recycle before completing the recycle loop. To avoid problems with rigorous tower simulations that are difficult to converge, one strategy is to include shortcut columns in the simulation that has a recycle loop. Then, simulate the towers rigorously outside of the recycle loop. This can be accomplished by copying the feed streams to the shortcut columns to the feed streams to the rigorous towers. However, it must be understood that if you change the process simulation with recycle, the contents of the shortcut column feed streams are not automatically copied to the feed streams of the rigorous tower. You must do this manually each time, and then you must rerun the simulation on the rigorous towers after having copied the streams.

Do not forget that this is a two-phase reaction, and this option must be selected in one the first screen for the kinetic reactor.

Major #2 - Confidentiality Statement

ChE 456
February 24, 2003

This is to certify that this written report and all of the work contained within it, regarding Major #2 in ChE 456, is the result of my own work. I have neither collaborated nor discussed this work with **anyone else**, other than the allowable purchasing of consulting time from the instructors. In addition, I agree not to discuss the contents of this project with **anyone** until after it has been reviewed by Professors Shaeiwitz and Turton in class.

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Student in ChE 456 February 24, 2003