

Design Project

Reaction Engineering and Separations

Drying Oil Production

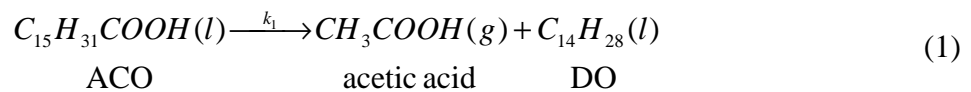
Drying oils are additives to paints and varnishes to aid in the drying process when these products are applied to surfaces. It has been determined that the market for drying oil in Southeast Asia is expanding. Therefore, we are planning to construct a new facility to increase capacity in that region. 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 plants in the United States. 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 $300^{\circ}C$ to avoid fouling due to excessive gum formation.

Reaction Kinetics

The reactions and reaction kinetics are as follows:



where

$$-r_1 = k_1 C_{ACO} \quad (3)$$

$$-r_2 = k_2 C_{DO}^2 \quad (4)$$

and

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

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

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

Specific Assignments

ChE 312

Determine the number of distillation columns required, their locations, their sequence, and enough information for each column to determine their costs. The distillation column that purifies the drying oil should be designed in detail. A detailed design of a tray tower includes number of trays, tray spacing, diameter, reflux ratio, active area, weir height, top and bottom pressure specifications, and design of auxiliary equipment (heat exchangers, pump, reflux drum, if present). A detailed design of a packed tower includes height, packing size and type, and the same other specifications as in a tray tower. For all columns in this project, you may assume that HETP = 0.6 m. For the distillation column, the better economical choice between a packed and tray tower should be determined. For either a packed or a tray distillation column, the optimum reflux ratio should be determined.

Note that a tower consists of a vessel with internals (trays or packing). The constraints on a vessel are typically a height-to-diameter ratio less than 20. However, it is possible to extend this ratio to 30 as long as the tower is less than about 3 ft (1 m) in diameter. For larger-diameter towers, stresses caused by wind limit the actual height. Extra supports are needed for a height-to-diameter ratio above 20, even for smaller diameter columns. Therefore, there is a capital cost “penalty” of an additional 25% (only on the vessel) up to a ratio of 25, and a “penalty” of an additional 100% up to a ratio of 30.

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 in the reboiler, 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 packing factor as defined in Wankat¹, p. 424, is that for Koch Flexipac #2. Assume the HETP for the structured packing to be 0.6 m (see the definition of HETP in Wankat¹, p. 418, and the relationship between HETP and H_{OG} in Equation 19.36 in Wankat¹), and that the pressure drop is 0.2 kPa/m (0.245 inch water/ft).

The gum filter should be simulated as a perfect separator. The capital cost of the vessel and filter is given by:

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

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

ChE 325

Three reactor types may be considered for use in this design. They are an adiabatic reactor, an “isothermal” reactor, and a reactor with heat exchange. An “isothermal” reactor is defined here as one with a specified outlet temperature, not necessarily the inlet temperature, and some form of heat exchange is needed to add or remove the heat of reaction to maintain constant temperature. Chemcad will model the entire reactor as “isothermal” at that temperature. It must be understood that this situation is not physically realistic. In a reactor with heat exchange, the temperature along the length of the packed-bed reactor is not constant. The temperature can be controlled by varying the temperature and flowrate of the heat-transfer fluid, heat-transfer area, and the catalyst/inert ratio. One suggestion for the heat-transfer fluid is Dowtherm™ A; however, you may make another choice, such as molten salt. If a heat-transfer fluid is used, it is circulated in a closed loop through the reactor where its temperature is increased (if the reaction is endothermic) or decreased (if the reaction is exothermic). Then, heat is added (removed) from the fluid in a heat exchanger (or fired heater, if needed). The heat-transfer fluid is then pumped back to the reactor. Properties of Dowtherm A™ are in Appendix 3.

For your best case, you should include a discussion of the temperature, pressure, and concentration profiles obtained from Chemcad.

General

The entire drying oil process should be optimized using decision variables of your choosing. Decision variables should be chosen as the design variables most strongly affecting the objective function. There are topological optimization and parametric optimization. In topological optimization, which is usually done first, the best process configuration is chosen. Parametric optimization involves varying operating variables and should be done after topological optimization is complete. Some examples of parameters that can be used as decision variables are reactor temperature, pressure, and conversion; absorber temperature and pressure; and distillation column reflux ratio.

Economic Analysis

When evaluating alternative cases, the equivalent annual operating cost (EAOC) objective function should be used. The EAOC is defined as

$$\text{EAOC} = -(\text{product value} - \text{feed cost} - \text{utility costs} - \text{waste treatment cost} - \text{capital cost annuity})$$

A negative EAOC means there is a profit. It is desirable to minimize the EAOC; i.e., a large negative EAOC is very desirable.

The capital cost annuity is an *annual* cost (like a car payment) associated with the *one-time*, fixed cost of plant construction.

The capital cost annuity is defined as follows:

$$\text{capital cost annuity} = FCI \frac{i(1+i)^n}{(1+i)^n - 1}$$

where *FCI* is the installed cost of all equipment; *i* is the interest rate (take $i = 0.15$) and *n* is the plant life for accounting purposes (take $n = 10$).

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:

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

Report Format

This report should conform to the Department 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 sample calculations. These calculations should be easy to follow.

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.

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, 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 discussion section pertinent to each class plus a general discussion section for optimization of the entire process
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 (packing) design specifications (if you use Chemcad to design the trays (packing)). It should not contain stream properties. Missing Chemcad output will not be requested; credit will be deducted as if the information is missing.

Other Information

Unless specifically stated in class, the information in this document is valid for this project only. Any information in the sophomore projects not specifically stated in this document is not valid for this project.

Deliverables

Each group must deliver a report (two identical copies, one for each professor) written using a word processor. The report should be clear and concise. The format is explained in the document *Written Design Reports*. Any report not containing a labeled PFD and a stream table, each in the appropriate format, will be considered unacceptable. PFDs from Chemcad are generally unsuitable unless you modify them significantly. When presenting results for different cases, graphs are superior to tables. For the optimal case, the report appendix should contain details of calculations that are easy to follow. There should be separate appendices for each class, ChE 312 and ChE 325, each containing calculations appropriate for the respective class. These may be handwritten if done so neatly. Calculations that cannot be easily followed will lose credit.

Each group will give an oral report in which the results of this project will be presented in a concise manner. The oral report should be between 15-20 minutes, and each group member must speak once. Reports exceeding this time limit will be stopped. A 5-10 minute question-and-answer session will follow. Instructions for presentation of oral reports are provided in a separate document entitled *Oral Reports*. The oral presentations will be Wednesday, April 21, 2004, starting at 11:00 a.m. and running until approximately 3:00 p.m. Attendance is required of all students during their classmates' presentations (this means in the room, not in the hall or the computer room). Failure to attend any of the above-required sessions will result in a decrease of one letter grade (per occurrence) from your project grade in ChE 312 and ChE 325.

The written project report is due by 11:00 a.m. Wednesday, April 21, 2004. Late projects will receive a minimum deduction of one letter grade.

In order to evaluate each team members writing skills, the results and discussion sections for each specific assignment should be written by a different team member. The authorship of each of these specific assignments should be clearly specified in the report. If a team has four members, the member not authoring a specific assignment should author the cover memorandum, abstract, introduction, and conclusion.

Revisions

As with any open-ended problem (*i.e.*, a problem with no single correct answer), the problem statement above is deliberately vague. The possibility exists that, as you work on this problem, your questions will require revisions and/or clarifications of the problem statement. You should be aware that these revisions/clarifications may be forthcoming.

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. 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 -CH₃ group, 25 >CH₂ groups, 1 =CH₂ 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.

Appendix 2 Economic Data

Equipment Costs (Purchased)

Note: The numbers following the attribute are the minimum and maximum values for that attribute. For a piece of equipment with a lower attribute value, use the minimum attribute value to compute the cost. For a piece of equipment with a larger attribute value, extrapolation is possible, but inaccurate. To err on the side of caution, you should use the price for multiple, identical smaller pieces of equipment.

Pumps	$\log_{10}(\text{purchased cost}) = 3.4 + 0.05\log_{10} W + 0.15[\log_{10} W]^2$ $W = \text{power (kW, 1, 300)}$ assume 80% efficiency
Heat Exchangers	$\log_{10}(\text{purchased cost}) = 4.6 - 0.3\log_{10} A + 0.8[\log_{10} A]^2$ $A = \text{heat exchange area (m}^2\text{, 10, 1000)}$
Compressors	$\log_{10}(\text{purchased cost}) = 2.3 + 1.4\log_{10} W - 0.1[\log_{10} W]^2$ $W = \text{power (kW, 450, 3000)}$ assume 70% efficiency
Compressor Drive	$\log_{10}(\text{purchased cost}) = 2.5 + 1.4\log_{10} W - 0.18[\log_{10} W]^2$ $W = \text{power (kW, 75, 2600)}$
Turbine	$\log_{10}(\text{purchased cost}) = 2.5 + 1.45\log_{10} W - 0.17[\log_{10} W]^2$ $W = \text{power (kW, 100, 4000)}$ assume 65% efficiency
Fired Heater	$\log_{10}(\text{purchased cost}) = 3.0 + 0.66\log_{10} Q + 0.02[\log_{10} Q]^2$ $Q = \text{duty (kW, 3000, 100,000)}$ assume 80% thermal efficiency assume can be designed to use any organic compound as a fuel
Vertical Vessel	$\log_{10}(\text{purchased cost}) = 3.5 + 0.45\log_{10} V + 0.11[\log_{10} V]^2$ $V = \text{volume of vessel (m}^3\text{, 0.3, 520)}$
Horizontal Vessel	$\log_{10}(\text{purchased cost}) = 3.5 + 0.38\log_{10} V + 0.09[\log_{10} V]^2$ $V = \text{volume of vessel (m}^3\text{, 0.1, 628)}$
Catalyst	\$2.25/kg

Packed Tower	Cost as vessel plus cost of packing
Packing	$\log_{10}(\text{purchased cost}) = 3 + 0.97 \log_{10} V + 0.0055 [\log_{10} V]^2$ $V = \text{packing volume (m}^3, 0.03, 628)$
Tray Tower	Cost as vessel plus cost of trays
Trays	$\log_{10}(\text{purchased cost}) = 3.3 + 0.46 \log_{10} A + 0.37 [\log_{10} A]^2$ $A = \text{tray area (m}^2, 0.07, 12.3)$
Storage Tank	$\log_{10}(\text{purchased cost}) = 5.0 - 0.5 \log_{10} V + 0.16 [\log_{10} V]^2$ $V = \text{volume (m}^3, 90, 30,000)$
Reactors	For this project, the reactor is considered to be a vessel.

It may be assumed that pipes and valves are included in the equipment cost factors. Location of key valves should be specified on the PFD.

Utility Costs

Low Pressure Steam (618 kPa saturated)	\$7.78/1000 kg
Medium Pressure Steam (1135 kPa saturated)	\$8.22/1000 kg
High Pressure Steam (4237 kPa saturated)	\$9.83/1000 kg
Natural Gas (446 kPa, 25°C)	\$6.00/GJ
Fuel Gas Credit	\$5.00/GJ
Electricity	\$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	\$2.45/1000 kg
Cooling Water	\$0.354/GJ
available at 516 kPa and 30°C	
return pressure ≥ 308 kPa	
return temperature is no more than 15°C above the inlet temperature	
Refrigerated Water	\$4.43/GJ
available at 516 kPa and 10°C	
return pressure ≥ 308 kPa	
return temperature is no higher than 20°C	

Deionized Water available at 5 bar and 30°C	\$1.00/1000 kg
Waste Treatment of Off-Gas	incinerated - take fuel credit
Refrigeration	\$7.89/GJ
Wastewater Treatment	\$56/1000 m ³

Any fuel gas purge may be assumed to be burned elsewhere in the plant at a credit of \$2.50/GJ. Steam produced cannot be returned to the steam supply system for the appropriate credit. Steam produced in excess of that required in this process is purged with no credit.

Equipment Cost Factors

Total Installed Cost = Purchased Cost (4 + material factor (MF) + pressure factor (PF))

Pressure < 10 atm, PF = 0.0	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects
(absolute) 10 - 20 atm, PF = 0.6	
20 - 40 atm, PF = 3.0	
40 - 50 atm, PR = 5.0	
50 - 100 atm, PF = 10	

Carbon Steel	MF = 0.0
Stainless Steel	MF = 4.0

Appendix 3 Other Design Data

Heat Exchangers

For heat exchangers, use the following approximations for heat-transfer coefficients to allow you to determine the heat transfer area:

situation	h (W/m ² °C)
condensing steam	6000
condensing organic	1000
boiling water	7500
boiling organic	1000
flowing liquid	600
flowing gas	60

Physical Properties of Dowtherm™ A

temperature use range (in liquid phase)	60°F – 750°F
vapor pressure at 750°F	137.8 psig
thermal conductivity (avg. over use range)	0.07 BTU/hr ft°F
heat capacity (avg. over use range)	0.5 BTU/lb°F
viscosity (at max. and min. temp. use range)	0.14 cp, 6.0 cp
density (avg. over use range)	54 lb/ft ³