

Separations and Reaction Engineering Spring 2000

Design Project

Production of Acetone

Process Objective Function

We would like to complete our investigation of the economic feasibility of producing 15,000 metric tons per year of 99.9 mol% acetone from isopropyl alcohol. It is unlikely that this process will appear profitable because most acetone is made as a byproduct of phenol manufacture. However, we expect to be able to charge a premium for our acetone since it will be free of aromatics. Therefore, your objective function should be the break-even price (BEP) for acetone, defined as follows:

$$\begin{aligned} & (\text{Acetone Produced per Year})(C_B) = \\ & \text{Annuity Value of Total Installed Cost} + \text{Annual Cost of Raw Materials} + \text{Annual Utility Cost} - \\ & \text{Annual Revenue from By-products} - \text{Annual Credit from Fuel Gas and Steam} \end{aligned}$$

where C_B is the break-even price for acetone

The above equation for estimating the cost of acetone is based on the minimum price for which acetone could be sold to cover our operating expenses. A 10-year plant lifetime ($n = 10$) and an interest rate of 15% ($i = 0.15$) should be used. The annuity value of the total installed cost is calculated by

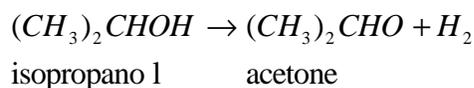
$$\text{annuity value} = \text{capital cost} \left[\frac{i(1+i)^n}{(1+i)^n - 1} \right]$$

In your final analysis, please compare your BEP for acetone to the current market price for acetone.

A process flow diagram (PFD) is not presented in this problem statement. You should be in a position to synthesize your own PFD based on your previous experience with this project.

Reaction Kinetics

The main reaction for producing acetone is



and the kinetics for this reaction are given below:

$$-r_{IPA} = k_1 C_{IPA} \frac{\text{mol IPA}}{\text{m}^3 \text{catalyst} \cdot \text{s}}$$

where

$$k_1 = 1.76 \times 10^5 \exp\left[-\frac{60,000}{RT}\right] \frac{\text{m}^3 \text{gas}}{\text{m}^3 \text{catalyst} \cdot \text{s}}$$

$$C_{IPA} = \frac{\text{mol IPA}}{\text{m}^3 \text{gas}}$$

These kinetics are only valid if the actual conversion does not exceed 85% of the equilibrium conversion at reactor conditions. Although, several side reactions are possible, none of them take place to any considerable extent. The activation energy in the kinetic expression above is in units of kJ/kmol.

Catalyst Information

Catalyst physical properties are given below:

density of the inert catalyst, $\rho_{ci} = 2500 \text{ kg/m}^3$

density of solid catalyst, $\rho_c = 2500 \text{ kg/m}^3$

packed bed voidage of the cylindrical pellets = 0.5

void fraction of the spherical particles at minimum fluidizing conditions = 0.55

particle diameter, $d_p = 100 \text{ }\mu\text{m}$

Chemcad Hints

For heat exchangers with multiple zones, it is recommended that you simulate each zone with a separate heat exchanger. Actual equipment may include several zones, so costing should be based on the actual equipment specifications. On your PFD, only the actual equipment should appear.

For the distillation columns, you should use the shortcut method (SHOR) to get estimates for the rigorous distillation simulation (TOWR or SCDS). The shortcut method may be used until an optimum case is near. It is then expected that everyone will obtain a final design using rigorous simulation of the columns. For an absorber, shortcut calculations are not possible.

When simulating a process using “fake” streams and equipment, it is absolutely necessary that the process flow sheet that you present not included any “fake” streams and equipment. It must represent the actual process.

Specific Assignments

General

Optimize the process using decision variables of your choosing. You should choose as decision variables the design variables most strongly affecting the objective function.

ChE 112 – Separations

Determine the number of distillation columns required, their location, and enough information for each distillation column to cost it. The distillation column that provides the acetone product should be designed in detail. Additionally, if you choose to recover acetone from the flash vaporizer vapor stream by scrubbing with water (must be deionized) or any other solvent, that absorber must 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.

ChE 172 – Reaction Engineering

Two reactors are to be considered for use in this design. They are a fluidized bed reactor and a packed bed reactor. The gas-phase, heterogeneous reaction to form acetone from isopropanol occurs with the use of a proprietary catalyst within the temperature range of 250°C to 475°C. In a packed bed, the temperature must not vary by more than $\pm 20^\circ\text{C}$ from the inlet temperature. Fortunately, the fluidized bed reactor may be assumed to be well mixed and isothermal, so it may operate at any temperature in the range stated above. The temperature distribution along the length of the packed bed reactor is not constant. It “can” be controlled by varying the temperature and flowrate of the heat transfer fluid, heat transfer area, and the catalyst/inert catalyst ratio. Other means to control the temperature distribution along the packed bed reactor length are possible and will receive extra credit if investigated. One suggestion for the heat transfer fluid is Dowtherm™ A; however, you may make another choice. The fluid is circulated in a closed loop through the fired heater and the reactor. Due to selectivity considerations, the maximum single-pass conversion in either type of reactor must not exceed 80% or 85% of the equilibrium conversion, whichever is smaller.

You must state why the packed bed or fluidized bed is chosen for your optimal design. The packed bed reactor must be designed in detail with Polymath, and the plot of your Polymath and Chemcad simulations must be compared on the same graph and discussed both in the body of your report and in the presentation. A disk must be provided with your final report that gives both Chemcad and Polymath simulations of the packed bed reactor at corresponding operating conditions.

Cost Data

Equipment Costs (Purchased)

Pumps	$\$630 (\text{power, kW})^{0.4}$
Heat Exchangers	$\$1030 (\text{area, m}^2)^{0.6}$
Compressors	$\$770 (\text{power, kW})^{0.96} + 400 (\text{power, kW})^{0.6}$
Turbine	$\$2.18 \times 10^5 (\text{power output, MW})^{0.6}$ assume 65% efficiency
Fired Heater	$\$635 (\text{duty, kW})^{0.8}$ assume 80% thermal efficiency assume can be designed to use any organic compound as a fuel
Vessels	$\$[1.67(0.959 + 0.041P - 8.3 \times 10^{-6}P^2)] \times 10^z$ $z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$ $D = \text{diameter, m } 0.3 \text{ m} < D < 4.0 \text{ m}$ $L = \text{height, m } L/D < 20$ $P = \text{absolute pressure, bar}$
Catalyst	$\$2.25/\text{kg}$
Reactor	packed bed: $\$3,000/\text{m}^2$ of heat transfer surface fluidized bed: $\$10,000/\text{m}^2$ of heat transfer surface
Packed Tower	Cost as vessel plus cost of packing
Packing	$\$(-110 + 675D + 338D^2)H^{0.97}$ $D = \text{vessel diameter, m; } H = \text{vessel height, m}$
Tray Tower	Cost as vessel plus cost of trays
Trays	$\$(187 + 20D + 61.5D^2)$ $D = \text{vessel diameter, m}$
Storage Tank	$\$1000V^{0.6}$ $V = \text{volume, m}^3$

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.

Raw Materials

isopropyl alcohol *see Chemical Market Reporter*

Products

acetone *see Chemical Market Reporter*

hydrogen (if purified) \$35/1000 std m³

Utility Costs

Low Pressure Steam (618 kPa saturated) \$6.62/1000 kg

Medium Pressure Steam (1135 kPa saturated) \$7.31/1000 kg

High Pressure Steam (4237 kPa saturated) \$8.65/1000 kg

Natural Gas (446 kPa, 25°C) \$3.00/GJ

Fuel Gas \$2.75/GJ

use this price for fuel gas credit

Electricity \$0.06/kW h

Boiler Feed Water (at 549 kPa, 90°C) \$2.54/1000 kg

Cooling Water \$0.16/GJ

available at 516 kPa and 30°C

return pressure \geq 308 kPa

return temperature is no more than 15°C above the inlet temperature

Refrigerated Water \$1.60/GJ

available at 516 kPa and 10°C

return pressure \geq 308 kPa

return temperature is no higher than 20°C

Deionized Water \$1.00/1000 kg

available at 5 bar and 30°C

Waste Treatment of Off-Gas incinerated - take fuel credit

Refrigeration

\$60/GJ

Equipment Cost Factors

Pressure (absolute)	< 10 atm, 0.0 10 - 20 atm, 0.6 20 - 40 atm, 3.0 40 - 50 atm, 5.0 50 - 100 atm, 10	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects
Carbon Steel	0.0	
Stainless Steel	4.0	

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

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

Other Information

You should assume that a year equals 8000 hours. This is about 330 days, which allows for periodic shutdown and maintenance.

Unless specifically stated in class, the information in this document is that which is valid for this project only. Any information in the sophomore projects not specifically stated in this document is invalid 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 112 and ChE 172, 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. 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 19, 2000 starting at 11:00 a.m. and running until approximately 3:00 p.m. It is possible that some presentations will be on Thursday, April 20, 2000, beginning at 11:00 am. 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 112 and ChE 172.

The written project report is due by 11:00 a.m. Wednesday, April 20, 2000. Late projects will receive a minimum of a one letter grade deduction.

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.