Reactors and Separations
Design Project

Production of Cumene

Process Objective Function

We must now complete gathering information that will allow our firm to enter the cumene market at an opportune time. To accomplish this goal, we request that your design team complete the estimate for the *minimum* price such that the construction and operation of a new plant, which will produce 100,000 metric tons/yr of cumene, will be profitable. Compare your calculated minimum cost for cumene with the current selling price. It can be found in the latest edition of the *Chemical Marketing Reporter* at the Evansdale Library along with the cost of the raw materials. Therefore, use the break-even price of cumene as the objective function to optimize your process. The equation to be used to estimate this price is given below:

(Cumene Produced per Year) (C_B) =
Annuity Value of Total Installed Cost + Annual Cost of Raw Materials + Annual Utility Cost - Annual Revenue from Byproducts - Annual Credit from Fuel Gas and Steam

where C_B is the break-even price for cumene

The above equation for estimating the cost of cumene is based on the minimum price that cumene could be sold for to cover our operating expenses. These economic details were introduced in ChE 38, and will be covered in more detail in ChE 182/183. You should use a 10-year plant lifetime and an interest rate of 15%.

Cumene Production Reaction

The kinetics for the reactions are given below. For the primary reaction:

$$\underset{propylene}{C_3H_6} + \underset{benzene}{C_6H_6} \xrightarrow{k_1} \underset{cumene}{C_9H_{12}}$$

$$r_1 = k_1 c_p c_b \quad \text{mole / g cat sec}$$

$$k_1 = 3.5 \times 10^4 \exp\left(\frac{-24.90}{RT}\right)$$

For the secondary reaction:

$$\underset{propylene}{C_3H_6} \quad + \quad \underset{cumene}{C_9H_{12}} \xrightarrow{k_2} \underset{p-diisopropyl\ benzene}{C_{12}H_{18}}$$

$$r_2 = k_2 c_p c_c \quad \text{mole / g cat sec}$$

$$k_2 = 2.9 \times 10^6 \exp\left(\frac{-35.08}{RT}\right)$$

where the units of the activation energy are kcal/mol, the units of concentration are mol/L, and the temperature is in Kelvin.

For a shell and tube packed bed, the recommended configuration, the following data may be assumed:

catalyst particle diameter d_p = 3 mm
catalyst particle density ρ_{cat} = 1600 kg/m^3
void fraction ε = 0.50
heat transfer coefficient from packed bed to tube wall h = 60 W/m^2°C
use standard tube sheet layouts as for a heat exchanger
if tube diameter is larger than in tube sheet layouts, assume that tube area is 1/3 of shell area

Assignment

General

Optimize the process using decision variables of your choosing. You should choose as decision variables the design variables which most strongly affect 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 benzene recycle should be designed in detail.

ChE 172 - Reactors

The reactor is a packed bed with either cocurrent or countercurrent cooling. Your design team must determine which reactor configuration is more economical and defend your choice in both the presentation and written report. Therefore, optimize the process for both reactor types. You must also choose and discuss your choice of decision variables. At no place along the length of the process side of the reactor will the temperature deviate from the inlet temperature by more than 20°C. Also, the reactor process side inlet temperature is constrained between 300°C and 400°C. A filler material is available which has the same density, diameter, void fraction, heat capacity, price, etc., of the catalyst. It is inert and may be installed within the reactor without catalyzing the reaction. Since Chemcad has no allowance for the Ergun equation hand estimate the pressure drop on the process side of the reactor and plug it into Chemcad for each simulation. Your design team must provide a copy of the design equations that include the Ergun equation, and plots of temperature, pressure, and concentrations of the chemical species verses reactor length for the optimal reactor design. Solve these equations using Polymath or another ordinary differential equation solver. Repeat this design/analysis for the other reactor type. Discuss/compare both the analytical and Chemcad design.

Chemcad Hints

Use SRK for the entire process.

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.

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.

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.

Cost Data

Raw Materials

Benzene (>99.9 wt% purity) — see *Chemical Marketing Reporter*

Propylene (£ 5 wt% propane impurity) — \$0.095/lb

Product

Cumene (>99 wt% purity) — see *Chemical Marketing Reporter*

Utility Costs

Low Pressure Steam (446 kPa saturated) — \$3.00/1000 kg

Medium Pressure Steam (1135 kPa saturated) — \$6.50/1000 kg

High Pressure Steam (4237 kPa saturated) — \$8.00/1000 kg

Natural Gas (446 kPa, 25°C) — \$3.00/10^6 kJ

Fuel Gas (446 kPa, 25°C) — \$2.75/10^6 kJ

Electricity — \$0.08/kWh

Boiler Feed Water (at 549 kPa, 90°C) — \$300.00/1000 m^3

Cooling Water — \$20.00/1000 m^3
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 — \$200.00/1000 m^3
available at 516 kPa and 10°C
return pressure ≥ 308 kPa
return temperature is no higher than 20°C

Waste Treatment — \$1/kg organic waste

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 = diameter, m $0.3\text{ m} < D < 4.0\text{ m}$ L = height, m $L/D < 20$ P = absolute pressure, bar
Catalyst	\$2.25/kg
Reactor	Cost as vessel with appropriate additional volume for cooling coil (fluidized bed) or tubes (shell and tube packed bed)
Packed Tower	Cost as vessel plus cost of packing
Packing	$\$(-110 + 675D + 338D^2)H^{0.97}$ D = vessel diameter, m; H = vessel height, m
Tray Tower	Cost as vessel plus cost of trays
Trays	$\$(187 + 20D + 61.5D^2)$ D = vessel diameter, m
Storage Tank	$\$1000V^{0.6}$ V = 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.

Equipment Cost Factors

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

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

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 written using a word processor. The report should be clear and concise. The format is explained in a separate document. 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 will be provided in a separate document. The oral presentations will be Wednesday, April 16, 1997 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 17, 1997, 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. Friday, April 17, 1997. 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.