Separations and Reaction Engineering

Design Project

Production of Styrene

We are continuing the feasibility study for the construction of a new, grass-roots, 100,000 metric ton/year, styrene plant. As part of the feasibility study, we require that you design a packed bed reactor and the separation section of the plant.

Styrene Production Reaction

During pilot plant runs, our research and development team determined that the catalyst we used last semester is easily poisoned and rendered ineffective. Therefore, it will not be utilized for our final design. Unfortunately, we must use another catalyst that has side reactions associated with its use. The reactions for styrene production using this new catalyst are as follows:

The reactions for styrene production for our new catalyst are as follows:

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \underset{2}{\overset{1}{\rightleftarrows}} \underset{\text{styrene}}{C_6H_5C_2H_3} + \underset{\text{hydrogen}}{H_2} \tag{1}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{3}{\longrightarrow} \underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \tag{2}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{hydrogen}}{H_2} \overset{4}{\longrightarrow} \underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{methane}}{CH_4} \tag{3}$$

Kinetics (subscripts on r refer to reactions in Equation (1) – (3):

$$r_1 = 8.44\times10^9 \exp\left(-\frac{35500}{RT}\right)p_{eb} \tag{4}$$

$$r_2 = 1503\exp\left(-\frac{5988}{RT}\right)p_{sty}\,p_{hyd} \tag{5}$$

$$r_3 = 7.21\times10^9 \exp\left(-\frac{57500}{RT}\right)p_{eb} \qquad (6)$$

$$r_4 = 2.09\times10^6 \exp\left(-\frac{43500}{RT}\right)p_{eb}\,p_{hyd} \qquad (7)$$

where p is in kPa, T is in K, R = 1.987 cal/mol K, and r_i is in mol/m^3 reactor s.

Assignment

Your first task is to develop a working base case flow sheet based on your design of last semester and the process changes listed in the reaction and separation sections of this assignment. In your oral report, you should discuss the important changes from this base case that result in significant impact on the process due to economic, safety, or environmental reasons. You should determine the Break-Even Price (BEP) for styrene that is at least 99% pure, for the base case. Then, you should consider any process modification that improves the BEP. We suggest that you use the BEP as an objective function for optimization for all of the work associated with this project. Full optimization is not required, but making no modifications should be considered unusual. The break-even price for 99% pure styrene product is calculated as follows:

$$\text{BEP} = \frac{CAP\left(\dfrac{i(1+i)^n}{(1+i)^n-1}\right) + \text{cost of reactants} + \text{operating costs - byproduct revenue}}{\text{kg styrene in crude product}}$$

Here, *CAP* is the installed capital cost of the entire process including feed tanks, n is the number of years of the project (10), and i is the cost of capital, 0.15 or 15%. The remainder of your assignment consists of the following:

1. Reaction Section (ChE 172)

The endothermic catalytic reaction takes place in multiple tubes of what, in appearance, resembles a single pass shell and tube heat exchanger. Our research and development team has determined that the catalyst will thermally deactivate when exposed to temperatures above 1100 K. Therefore, the maximum temperature of the catalyst at any point along the length of the reactor must not exceed 1000 K. Also, due to the thermal expansion effects, the maximum deviation between the upper and lower temperature of the catalyst along the reactor length must differ by no more than 50 K. To avoid hydrogen attack, all process components that contact hydrogen must be fabricated of a special steel consisting of 1.5 % chrome and 0.5% molybdenum.

Your choice of the decision variables you choose to optimize the reactor and process is your prerogative. However, at a minimum you are to complete the following tasks:

1. The reactor should be heated by either co-current or counter current heat exchange. Determine which case is better and state your reasoning during your presentation and in your design report.

2. Determine the optimal temperature for reactor operation.

3. Determine the optimal reactor pressure.

4. Design the reactor in full detail using both Chemcad and Polymath for a representative operating condition. Though this does not have to be your optimal condition, do not choose a condition that oversimplifies your problem. Show plots of the concentration of all of the individual chemical species, reactor temperature, and coolant temperature versus reactor length for the case of co-current heating. Discuss in detail in both your report and presentation reasons why the Chemcad and Polymath solutions differ. List the equations used in your Polymath program in the Appendix. You must provide an explanation of the nomenclature used for the program.

   The cost of the reactor should be taken as three times the cost of a regular vessel with the additional cost of catalyst at $200/(kg-year) and inert filler catalyst at $25/(kg-year). Both the catalyst and filler catalyst have a bulk density of 1282 kg/m^3 and a solid volume fraction of 0.6. Catalyst particles are spherically shaped and have a mean diameter of one (1) cm.

2. Separation Section (ChE 112)

Due to the additional side reactions that take place with the new catalyst, the separation section must be upgraded. The overhead from the three-phase separator contains hydrogen, ethylene and methane, which are used as fuel. Waste water exits out the bottom of the separator. Ethylbenzene, styrene, benzene, and toluene exit with the liquid organic. The first Tower=s overhead product consists of a minimum 99 % pure benzene/toluene mixture, which is sold to a local chemical plant at one-half the value of the pure components as found in the *Chemical Market Reporter*. The bottom product of that tower contains styrene and ethylbenzene. These products are further separated by a downstream tower that has styrene exiting as the bottom product and ethylbenzene exiting as the overhead product. Ethylbenzene is recycled as reactant to the process feed.

The three-phase flash can be simulated using the regular flash unit with three exit streams. All that is required is that you specify two outlet conditions. Since there is no heat transfer in this device, you should use the mode where the outlet temperature and pressure are identical to the inlet values. Any light gases not entering the top stream may be assumed to be vented from the reflux drum of the first tower and mixed with the hydrogen/light-gas steam before compression. This may be simulated with a component separator prior to the first tower, but the actual PFD should show the vent on the reflux drum.

It should be assumed that the minimum pressure required for all steams leaving the process to reach their destination is 2 bar.

The choice of the decision variables you choose to optimize the separation section and process is your prerogative. However, at a minimum you are to complete the following tasks:

1. Design the styrene purification tower in full detail. Make sure that there are no problems associated with flooding or weeping. Also, the pressure balance along the tower should reflect the proper use of available coolants or heating agents for the reflux and reboiler, respectively.

2. Determine the optimal pressure, and reflux ratio of the reflux returning to the top of styrene purification tower.

3. Towers other than the one designed in full detail need only be designed in enough detail to obtain a cost and to determine that flooding or weeping are not occurring.

Cost Data

Raw Materials

Ethylbenzene see value in *Chemical Market Reporter*

Product

Styrene	see value in *Chemical Market Reporter*
Benzene	one half value in *Chemical Market Reporter*
Toluene	one half value in *Chemical Market Reporter*

Utility Costs

Low Pressure Steam (618 kPa saturated)	$6.62/1000 kg
Medium Pressure Steam (1135 kPa saturated)	$7.31/1000 kg
Medium Pressure Steam (4237 kPa saturated)	$8.65/1000 kg
Natural Gas (446 kPa, 26°C)	$3.00/GJ
Fuel Gas (use this price for fuel gas credit)	$2.75/GJ
Electricity	$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	$2.54/1000 kg
Cooling Water available at 516 kPa and 30°C return pressure ∃308 kPa return temperature is no more than 15°C above the inlet temperature	$0.16/GJ
Refrigerated Water available at 516 kPa and 10°C return pressure ∃308 kPa return temperature is no more than 20°C	$1.60/GJ
Deionized Water available at 5 bar and 30°C	$1.00/1000 kg
Wastewater Treatment	$50/1000 m^3

Equipment Cost (Purchased)

Piping	\$/m=5.0 (diameter, in)
Valves	\$100 (flow diameter, in)$^{0.8}$ for control valve with orifice plate, double the price
Pumps	\$630(power, kW)$^{0.4}$
Heat Exchangers	\$1030 (area, m^2)$^{0.6}$ add 25% additional for boilers or evaporators
Compressors	\$770 (power, kW)$^{0.96}$ + \$400 (power, kW)$^{0.6}$ assume 65% efficiency
Turbine	\$2.18x10^5(power output, MW)$^{0.6}$ assume 65% efficiency
Fired Heater	\$635 (duty, kW)$^{0.8}$ assume 80% thermal efficiency assume unit can be designed to use any organic compound as a fuel
Vessels	\$[1.67(0.959 + 0.041P - 8.3x10^{-6} P^2)] x 10^z z = (3.17 + 0.2D + 0.5 $\log_{10}L$ + 0.21 $\log_{10}L^2$) D = diameter, m 0.3 m < L/D < 20 P = absolute pressure, bar
Reactor	See Reactor Assignment Section
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) D = vessel diameter, m
Storage Tank	\$ 1000 $V^{0.6}$ V = volume, m^3

Equipment Cost Factors

Pressure 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

Material Factors

Carbon Steel	0.0
Carbon Steel Containing, 1.5% Cr, 0.5% Mo	1.5
Stainless Steel	4.0

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

Heat Exchangers

Use the following approximations for heat transfer coefficients to allow you to determine the heat transfer area and heat exchanger cost.

Fluid	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 valid for this project only. Any information in the sophomore or first semester junior projects not specifically stated in this document is not valid for this project.

Deliverables

Each group must deliver a report written using a word processor. Two identical copies should be submitted, one for each instructor. The written project reports are due by 11:00 a.m. Wednesday, April 18, 2001. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. For the correct formatting information, refer to the document entitled *Written Design Reports*. Any report not containing a labeled PFD and a stream table, each in the appropriate format, will be considered unacceptable. Process Flow Diagrams from CHEM CAD 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 Amini-design.≅ These may be hand-written if done neatly. Calculations that cannot be easily followed will lose credit.

Since this project involves Amini-designs,≅ it is suggested that the report be organized as follows. There should be a general abstract and introduction. Then, there should be a results section followed by a discussion section for each Amin-design.≅ General conclusion and recommendation sections should follow. Process modifications and improvements from the base case unrelated to the mini-designs should be discussed in a combined result and discussion section entitled *Process Topology Modifications*. At a minimum, there should be an appendix for each of the Amini-designs.≅ However, this is not required for the Process Topology Modifications section. With this organization, there is no need for a separate section of the report for each class, as suggested in the document entitled *Written Design Reports.*

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. Each group member should speak only once. A 5-10 minute question-and-answer session will follow, and all members must participate. Refer to the document entitled *Oral Reports* for instructions. 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.*

Groups

You will do this project in a group of four. Since there are 28 students doing the project, there will be 7 groups 4.

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 clarification of the problem statement. You should be aware that these revisions/clarification may be forthcoming.