Fluid Mechanics, Heat Transfer, Thermodynamics

Design Project

Production of Styrene

We are investigating the feasibility of constructing a new, grass-roots, 100,000 metric tons/year, styrene plant. As part of the feasibility study, we would like you to investigate some of the details of the feed and reaction sections of the proposed plant.

Styrene Production Reaction

We have developed a new catalyst that suppresses all side reactions. Therefore, the only reaction is given below.

$$\underset{\text{ehylbenzene}}{C_6H_5CH_2CH_3} \rightleftarrows \underset{\text{styrene}}{C_6H_5CH=CH_2} + H_2 \qquad (1)$$

For the purposes of this preliminary evaluation, it is assumed that the reaction occurs in an adiabatic packed bed of catalyst particles. Practical equipment limitations make the maximum possible conversion 80% of the equilibrium conversion.

Feed and Reaction Sections

The PFD for the feed and reaction sections is given in Figure 1. Feed to the process consisting of liquid ethylbenzene, is mixed with recycle liquid ethylbenzene.

The reaction is endothermic and the reactor is adiabatic. The only constraint is a maximum temperature of 1000 K. If at a later point, if you want to make the reaction isothermal, heat may be added to the reactor by a molten salt heated in a furnace. The molten salt would be circulated in a loop from the furnace through the reactor. (Molten salt properties: C_p = 0.373 BTU/lb°F, k = 0.35 BTU/hr ft^2°F, ∓ = 1.7 cp, and → = 123 lb/ft^3) Following the reactor, the reaction products are cooled to the three-phase flash conditions. In the three-phase flash, hydrogen and wastewater are separated from the organics. Ethylbenzene and styrene are separated in a distillation column, which you may assume to be a perfect separator for this semester's project only. Any residual hydrogen and water entering the distillation column can easily be separated in the reflux drum (not shown) and added to either Stream 9 or Steram 11 (with appropriate pumping or compression). The hydrogen and wastewater streams must be at 2 bar for further treatment.

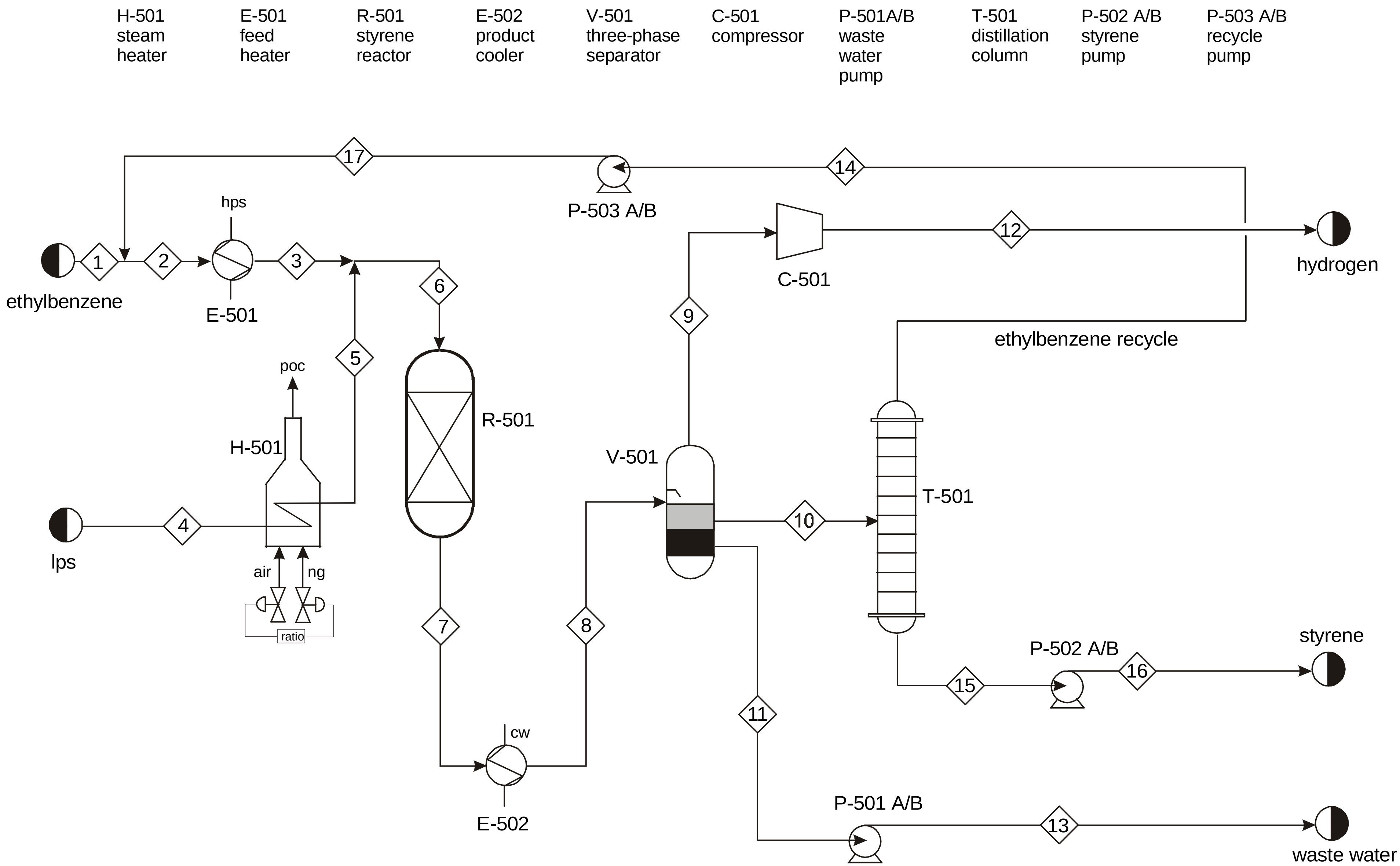

Figure 1: Unit 500: Production of Styrene from Ethylbenzene

Process Details

Feed Streams

Stream 1: ethylbenzene liquid at 210 kPa, 136°C

Stream 17: recycle ethylbenzene, at 210 kPa, temperature is that of saturated liquid at pressure of distillation column, which is 60 kPa

Effluent Streams

Stream 12: Hydrogen byproduct, must be at 200 kPa, do not consider purification and sale in this project

Stream 13: Wastewater stream to treatment, must be at 200 kPa

Stream 16: Styrene product, must be at 200 kPa

Equipment Summary

H-501: Fired Heater – a furnace that can heat to temperatures above high-pressure steam using an open flame

E-501: Heat Exchanger – to preheat ethylbenzene feed

R-501: Reactor – adiabatic

E-502: Product cooler

V-501: Three-phase separator – produces an oil-water-gas three-phase mixture that is assumed to separate easily into three distinct streams – can be simulated on Chemcad using flash – specify outlet T and P (outlet T must be inlet T), outlet P can be adjusted if valve added before flash

C-501: Compressor – to compress hydrogen to the required pressure

P-501: Pump – to pump waste water to required pressure – A/B means two in parallel with only one operating

P-502: Pump – to pump styrene product to required pressure – A/B means two in parallel with only one operating

P-503: Pump – to pump ethylbenzene recycle to required pressure – A/B means two in parallel with only one operating

T-501: Distillation column – to produce styrene product and ethylbenzene for recycle – use the component separator on Chemcad – assume there is no hydrogen in the feed even though the flash will show a small amount remaining – you may assume a perfect separator (which is physically impossible) for this semester only, *i.e.*, all ethylbenzene to the recycle and all styrene to the product

Assignment

The first task is to obtain base-case stream flows for the process using the conditions your group recommended in the Spring 2000 design. If your current group is a combination of multiple groups, just choose one set of results as a starting point. You may use Chemcad for this calculation, or you may use a spreadsheet. It is your choice.

The remainder of your assignment consists of three "mini-designs."

1. **Optimization of the Feed Section and Wastewater Pump.** (ChE 110) Refer to Figure 1. You are to size P-501 A/B. Determine the optimum pipe size for Streams 11 and 13. The objective function for the optimization is the Equivalent Annual Operating Cost (EAOC) of the pipe in Streams 11 and 13 and P-501 A/B ($/y). The *EAOC* is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + \text{annual operating costs for the P-501 A/B} \quad (2)$$

where *CAP* = the installed cost of P-501 A/B and the pipe in Stream 11

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \quad (3)$$

where i = 0.15 (15% rate of return) and n = 10 (ten-year plant life).

Do not include raw material costs, so *CAP* includes only the installed cost of pipes and pumps, and operating costs include the electricity to run the pump. Specify the liquid level to be maintained in V-501 to avoid cavitation of P-501 A/B. The pump P-501 A/B is 5 m horizontally distant from the V-501 draw. There are two 90° elbows. We have a supply of centrifugal pumps used in other plants. Their pump curves and their NPSH curves are attached (Figures 2 and 3). We would like the flexibility for 30% scale-up in the future.

You should also do a pressure analysis of the Streams 1 through 8 to make sure all pressures balance. Valves, pumps, compressors, and separators must be added as needed. It may be assumed that each stream has a pressure drop of 5 kPa. Heat exchangers that are not designed may be assumed to have a pressure drop of 30 kPa, and the reactor pressure drop may be assumed to be 25 kPa. (Note: We could make you calculate this by

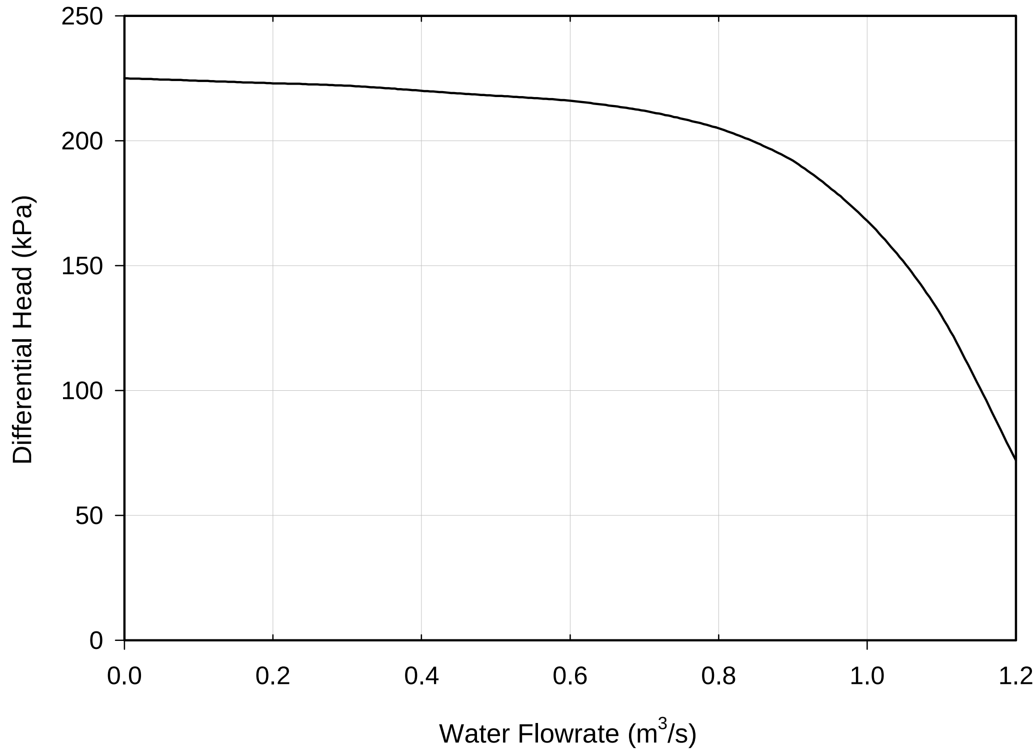

Figure 2: Pump Curve for P-501 A/B

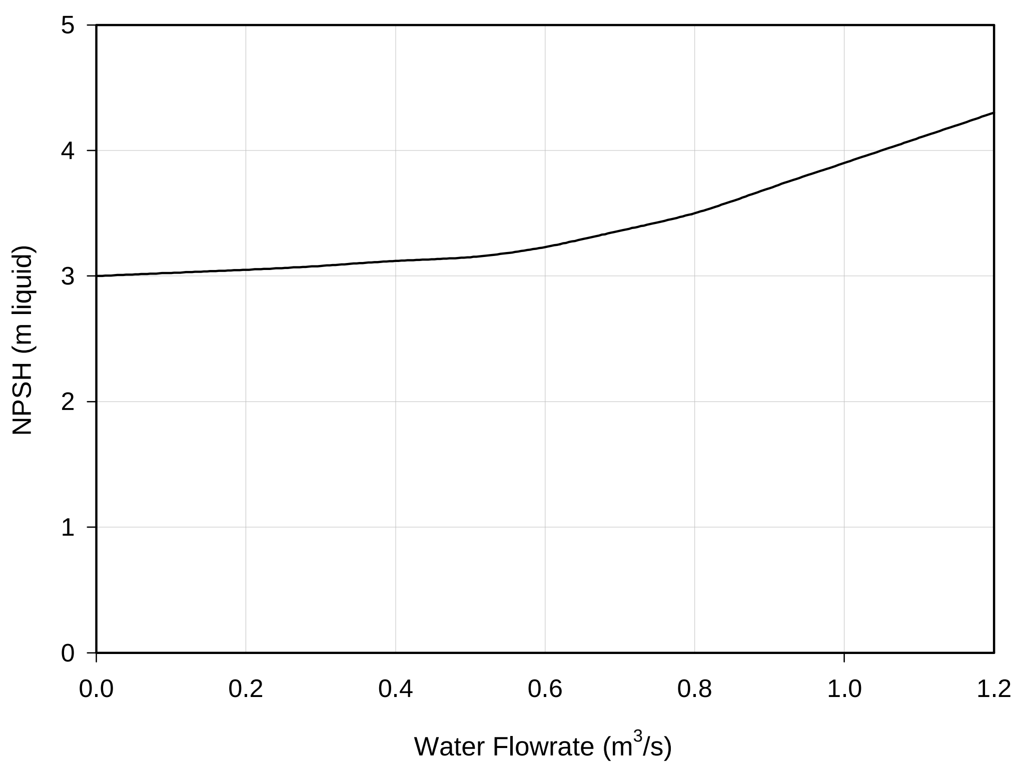

Figure 3: NPSH Curve for P-501 A/B

giving you details of the packing and the size of the reactor; however, we think you already have enough to do.)

Finally, determine the optimum pipe size for Stream 9. The pressure drop from V-501 to the compressor inlet is 10 kPa. Be certain that you do this analysis correctly.

2. **Design of E-501.** (ChE 111) The heat exchanger, E-501, must be designed in detail for the base case. The outlet pressure must be as specified, so the pressure drop in E-501 must be consistent with the feed-section pressure analysis discussed above.

3. **Determination of Break-even Price (BEP) for Crude Styrene.** (all classes, but mostly thermodynamics) A Chemcad simulation for your base case should be presented. The base case includes your chosen reactor and three-phase flash conditions. You should determine the BEP for crude styrene for the base case. Then, you should consider any process modifications that improve the BEP. Full optimization is not required, but making no modifications should be considered unusual. These modifications may be in equipment and/or process conditions such as reactor temperature, pressure, steam/ethylbenzene ratio, conversion, or flash temperature and pressure. The break-even price for crude styrene product is calculated as follows:

$$BEP = \frac{CAP\left(\frac{A}{P}, i, n\right) + \text{cost of reactants} + \text{operating costs} - \text{byproduct revenue}}{\text{kg styrene in crude product}} \qquad (4)$$

where *CAP* is now the installed capital cost for the entire feed and reaction sections, including the feed tanks. For this case, ignore the cost of the distillation column. The crude styrene product is actually the contents of Stream 10. Your discussion for this section should emphasize any differences in recommended operating conditions based on the inclusion of equipment costs and other practical matters.

Cost Data

Raw Materials

Ethylbenzene	see *Chemical Market Reporter*

Product

Styrene	see *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
High Pressure Steam (4237 kPa saturated)	\$8.65/1000 kg
Natural Gas (446 kPa, 25°C)	\$3.00/GJ
Fuel Gas use this price for fuel gas credit	\$2.75/GJ
Electricity	\$0.06/kW h
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 higher 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 Costs (Purchased)

Piping	\$/m = 5.0 (diameter, in)
Valves	$\$100\ (\text{flow diameter, in})^{0.8}$ for control valve with orifice plate, double the price
Pumps	$\$630\ (\text{power, kW})^{0.4}$
Heat Exchangers	$\$1030\ (\text{area, m}^2)^{0.6}$ add 25% additional for boilers or evaporators
Compressors	$\$770\ (\text{power, kW})^{0.96} + \$400\ (\text{power, kW})^{0.6}$ assume 70% efficiency
Turbine	$\$2.18 \quad 10^5\ (\text{power output, MW})^{0.6}$ 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	$\$[1.67(0.959 + 0.041P - 8.3 \quad 10^{-6}P^2)] \quad 10^z$ $z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$ D = diameter, m $0.3\text{ m} < D < 4.0\text{ m}$ L = height, m $3 < L/D < 20$ P = absolute pressure, bar
Reactor	assume to be \$1 million
Separator	if added to feed section – \$50,000 per separator

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
Stainless Steel	4.0

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

Heat Exchangers

For heat exchangers that do not have to be designed in detail, use the following approximations for heat transfer coefficients to allow you to determine the heat transfer area and heat exchanger cost.

situation	***h*** **(W/m²°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 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. Three identical copies should be submitted, one for each instructor. The written project reports are due by 11:00 a.m. Thursday, November 30, 2000. 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. 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 “mini-design.” These may be hand written if done neatly. Calculations that cannot be easily followed will lose credit.

Since this project involves “mini-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 “mini-design.” General conclusion and recommendation sections should follow. At a minimum, there should be an appendix for each of the “mini-designs.” 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. The oral presentations will be November 30, 2000, from 11:00 a.m. to 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 110, ChE 111, and ChE 142***.

Groups

You may do this project in a group of three or four. You should select your own group members. Since there are 25 students doing the project, there will be 7 groups. There will be 4 groups of 4 and 3 groups of 3.

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.