Fluid Mechanics, Heat Transfer, Thermodynamics Design Project

Production of Cumene

Process Objective Function

We are interested in 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 estimate the <u>minimum</u> price for cumene 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 price that cumene would have to be sold for in order for the price to "break-even." 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 reaction for cumene production from benzene and propylene is as follows:

$$C_3H_6 \quad + \quad C_6H_6 \quad \rightarrow \quad C_9H_{12}$$
propylene benzene cumene
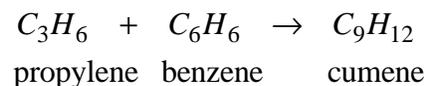
Process Description

The raw materials are benzene and propylene. Benzene and propylene are fed from separate storage tanks (TK-201 and TK-202, not shown on the PFD (Figure 1)), through pumps P-201 and P-202, to be heated by the fired heater (H-201). The storage tanks are operated at ambient temperature, which is assumed to reach a maximum of 43°C, but not

necessarily at ambient pressure. Two fuels are available for the fired heater. They are natural gas and the fuel gas by-product of the process. The process feed to the reactor (R-201) consists of 75% excess benzene. In the reactor, benzene and propylene react in an isothermal, exothermic reaction to form cumene. The reactor temperature is held at its isothermal value by internal heat exchange with boiler feed water. The process discharge of the reactor is fed to a heat exchanger (E-201) in which Stream 8 is cooled. Stream 9 is fed to the flash vessel (V-201) where the majority of the unreacted propylene and propane, and small amounts of other components, are discharged overhead as fuel gas and the bottoms discharge (Stream 11) consists of the remaining chemical components. The heat exchanger (E-201) and flash vessel (V-201) may operate at any pressure and/or temperature below the exit conditions of the reactor. You should add additional equipment as needed to effect this result. Stream 11 is then fed to the T-201 distillation column. At least 90 wt. % of the cumene in Steam 11 exits as product in Steam 12 and at least 90 wt.% of the benzene from Stream 11 exits with the overhead recycle stream. The plant must produce at least 100,000 metric tons/yr of the cumene product stream. Thise stream must exceed a weight specification of 99 wt.% cumene.

Process Details

Feed Streams

Stream 1:   benzene, pure liquid

Stream 2:   propylene with 5 wt.% propane impurity ($0.095/lb)

Effluent Streams

Stream 10:   fuel gas stream, a credit may be taken for the fuel gas or it may be reused in the process as fuel for H-201

Stream 12:   cumene product, at least 99.0 wt.% cumene

Equipment

Pump P-201:   The pump increases pressure of the benzene from the TK-201 benzene storage tank. The pump curves are shown in Figure 2.

Pump P-202:   The pump increases pressure of the propylene from the TK-202 propylene storage tank. The pump curves are shown in Figure 3.

Fired Heater H-201:   The fired heater heats Stream 6 until it is a vapor at the reactor feed conditions. H-201 is fueled by a mixture of air and either fuel gas or natural gas.
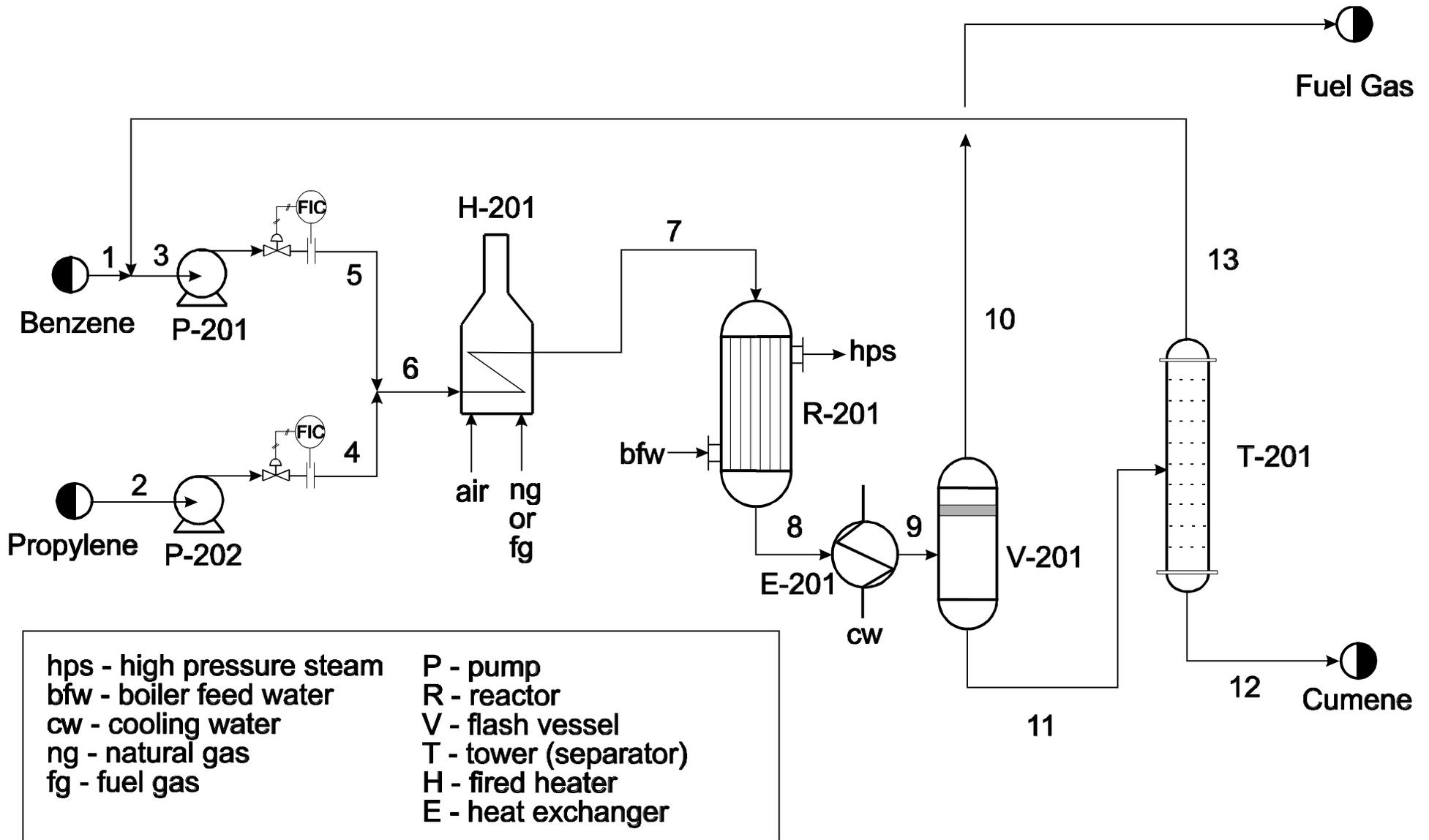
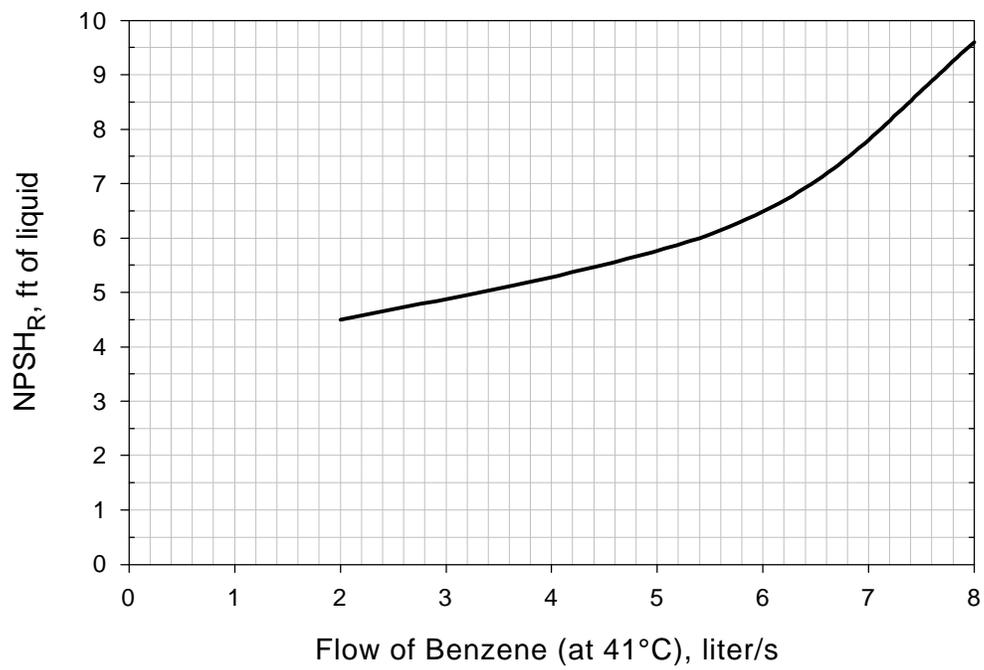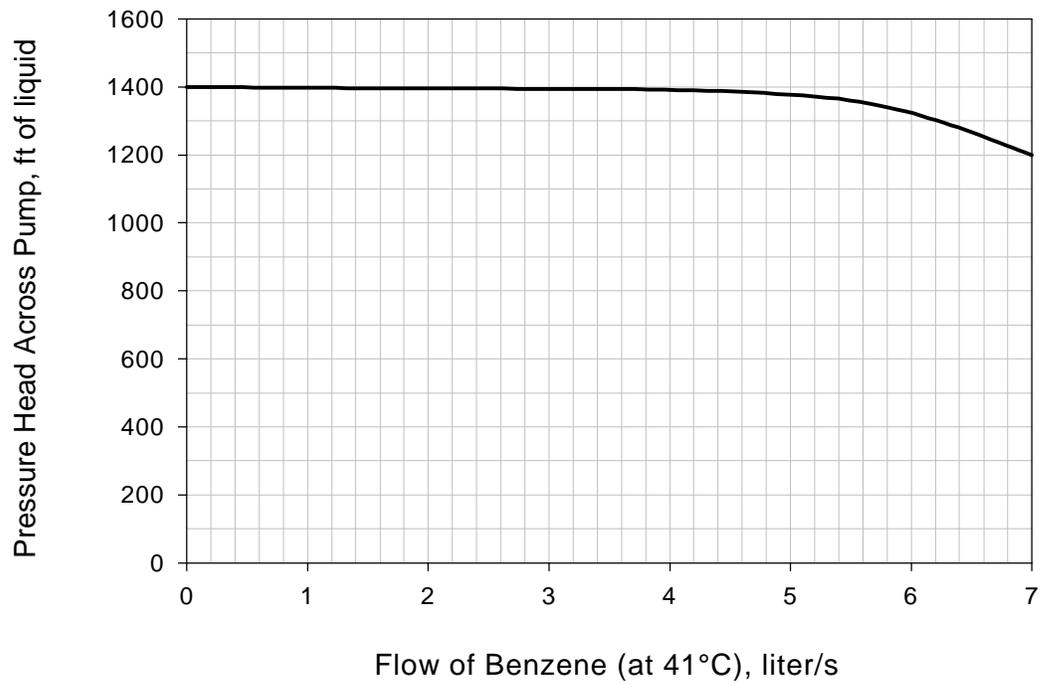Figure 1: Process Flowsheet for Cumene Production
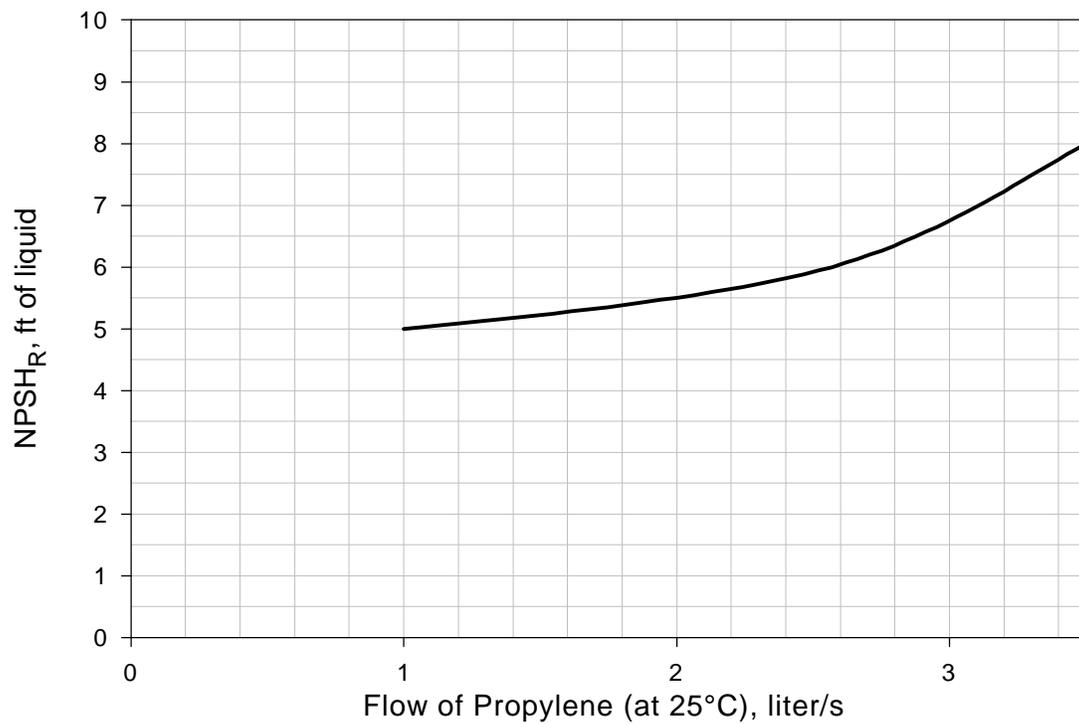
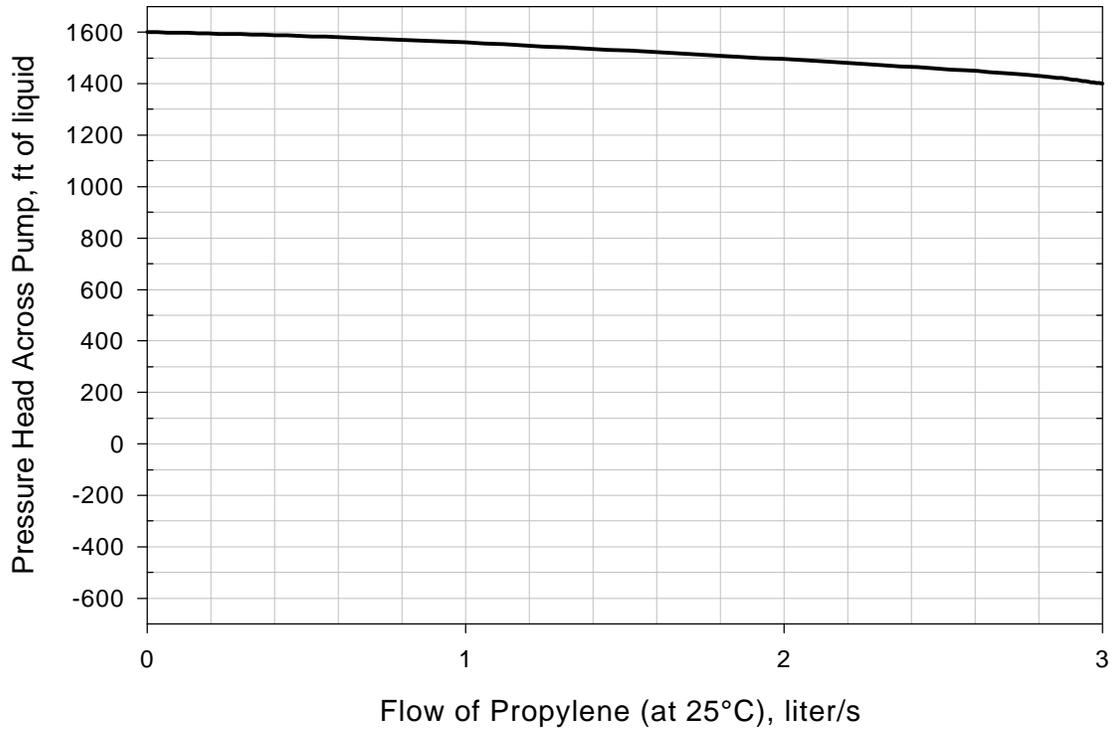Figure 2: Pump and NPSH Curves for P-201 A/B

Figure 3: Pump and NPSH Curves for P-202 A/B

Storage Tank TK-201: The tank stores a three-day supply of benzene as a pure liquid at ambient temperature. It is designed to withstand a pressure of 1.25 times the maximum operating pressure. The ambient temperature is assumed to reach a maximum of 43°C.

Storage Tank TK-202: The tank stores a three-day supply of the "impure" propylene at ambient temperature as a vapor/liquid mixture. It is bullet shaped and designed to withstand a pressure of 1.75 times the maximum operating pressure. It is installed horizontally on its longer side. The ambient temperature is assumed to reach a maximum of 43°C.

Heat Exchanger E-201: This heat exchanger cools or heats the discharge of reactor R-201.

Flash Vessel V-201: The vessel separates the light components of Stream 8 from the heavy components. Assume the separation is adiabatic.

Distillation Column T-201: The column separates cumene from benzene.

Reactor R-201: The reactor should be assumed to operate isothermally at 350°C along its length and at an entrance pressure of 3000 kPa. These conditions are required for optimal catalyst activity and should not be changed. At these conditions, the per-pass conversion of propylene equals 0.92.

Assignment

ChE 142 - Thermodynamics

1. A. Optimize the process using the pressure and temperature of flash vessel V-201 as the decision variables. Assume that all vapor streams behave as ideal gases and all liquid streams behave as ideal mixtures. This means that Raoult's Law can be used for V-201.

   B. Using the optimum conditions reported from Part A, redo your calculations based on non- ideal conditions. Recalculate the actual break-even cost and the actual production rate of the cumene using the operating conditions and feed flow rates of Part 1A.

   C. Provide detailed hand calculations that verify the performance of the flash vessel for ideal fluid phase equilibria of Part 1A and for the non-ideal conditions of Part 1B.

ChE 110 – Fluid Mechanics

2. A. Design the pipe network that includes storage tanks TK-201, TK-202, and Streams 1-6. You must specify the dimensions of the storage tanks, and the optimal pipe sizes subject to the constraints of the pump curves. The *H/D* (height/diameter) ratio of the tank TK-201 must fall within the range of 0.3 to 0.8, and the *L/D* (length/diameter) for tank TK-202 must fall within the range of 5.0 to 1.0. Given the pump curves shown in Figures 2 and 3, calculate the pump power requirements. Make sure that the $NPSH_A$ is sufficient for operation of the pumps. You must show all calculations, including a drawing of the system and $NPSH_A$ curves directly on the pump curve or facsimile. The system should be capable of operation at flows that are ± 25% of the design production rates. Equivalent pipe lengths should be taken as follows:

Stream #	Equivalent Length
1	25
2	35
3	10
4	40
5	40
6	50

   B. Show where you would place a control valve or valves and orifice plates in the feed section to control the flow of the reactants. Assume that the pressure drop due to each orifice plate is 20 inches of water. You must make sure the mechanical integrity of the pipe network is not compromised.

   C. Calculate the pressure drop across the packed bed reactor R-201. The reactor has a volume of 5 m³. Our specifications require that the *L/D* (length/diameter) ratio for the reactor fall between 0.5 and 3. Catalyst pellets are available in sizes of 0.1 mm, 1 mm, and 10 mm. The density of the catalyst is 1600 kg/m³ and the void fraction throughout the reactor is fixed at 0.4.

ChE 111 – Heat Transfer

3.   E-201 must be designed in detail, including tube size and pitch, baffle spacing, shell diameter, detailed pressure-drop calculations, etc. Pressure drops for heat exchangers other than E-201 may be estimated as 30 kPa for the tube side and 20 kPa for the shell side. Individual heat transfer coefficients for heat exchangers other than E-201 may be estimated as follows:

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

Utility Costs and Credits

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

Electricity $0.08/kWh

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

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

Cooling Water $20.00/1000 m^3
available at 516 kPa and 30°C
return pressure at 308 kPa

The return temperature should be no more than 15°C above the inlet temperature, otherwise there is an additional cost of $0.35/10^6 kJ

Refrigerated Water $200.00/1000 m^3
available at 516 kPa and 10°C
return pressure at 308 kPa
return temperature is no higher than 20°C
if return temperature is above 20°C, there is an additional cost of $7.00/10^6 kJ

Equipment Costs (Purchased):
(Based on Carbon Steel)

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}$
                    If extended surfaces are used, area is that for same size tubing without fins. Then add a 25% surcharge for fins.

Compressors $770 (power, kW)$^{0.96}$ + 400 (power, kW)$^{0.6}$

Steam Turbine $2.18 X 10^5 (power output, MW)$^{0.67}$
                    assume 75% efficiency

Fired Heater $635 (duty, kW)$^{0.8}$
                    assume 80% thermal efficiency

Reactor R-201 $250,000

Storage Tank $1000V$^{0.6}$
                    V = volume, m^3

Vessels $[1.67(0.959 + 0.041P - 8.3X10^{-6}P^2)] ´ 10^z
                    $z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$
                    D = diameter, m   0.3 m < D < 4.0 m
                    L = height, m   L/D < 20
                    P = pressure, bar

                    size vessels for 10 min liquid residence time based on being half-full of liquid

Equipment Cost Factors

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

Pressure (atm absolute)	Pressure Factor	
	0 - 10 1.0	does not apply to R-201 reactor, packing, trays or catalyst since their cost equations include pressure effects
1 - 10	0.0	
10 - 20	0.6	
20 - 40	3.0	
40 - 50	5.0	
50 - 100	10.0	

Material	Material Factor
Carbon Steel	0.0
1/2 Cr-1/2 Mo.	2.0
Stainless Steel	4.0

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. Information contained in this document will not necessarily be valid for next semester's project. You should feel free to look up other information from other sources.

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 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 110, ChE 111, and ChE 142, 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 Thursday, November 21, 1996 starting at 11:00 a.m. and running until approximately 4:00 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. Individuals with classes at 2:30 p.m. will have their groups' presentation scheduled first, and are excused from attending presentations after 2:00 p.m..

The written project report is due by 11:00 a.m. Friday, November 22, 1996. 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.