Fluid Mechanics, Heat Transfer, Thermodynamics Design Project

Production of Allyl Chloride

We are investigating the feasibility of constructing a new, grass-roots, 20,000 metric tons/year, allyl chloride production facility. The plant is to be built in La Nueva Cantina, Mexico based on the designs of our existing plants in Beaumont, TX and Mobile, AL. The Mexico site is favored because of its proximity to one of our propylene plants and local chlorine suppliers. As part of the feasibility study, we would like you to investigate some of the details of the reaction and refrigeration sections of the proposed plant.

Allyl Chloride Production Reactions

The reactions are given below. The primary reaction is:

$$C_3H_6 \quad + \quad Cl_2 \rightarrow \underset{allyl\ chloride}{C_3H_5Cl} \quad + \quad HCl$$

The secondary reactions are:

$$C_3H_6 \quad + \quad Cl_2 \rightarrow \underset{2-chloropropene}{C_3H_5Cl} \quad + \quad HCl$$

$$C_3H_6 \quad + \quad 2Cl_2 \rightarrow \underset{dichloropropene}{C_3H_4Cl_2} \quad + \quad 2HCl$$

$$C_3H_6 \quad + \quad 3Cl_2 \rightarrow \underset{carbon}{3C} \quad + \quad 6HCl$$

For the purposes of this preliminary evaluation, it is assumed that the reactions occur in a fluidized bed. The fluidized material is sand which scavenges any carbon formed. The sand is regenerated by recovering it with a cyclone and burning the carbon off with air in a combustion reaction. It may be assumed that the carbon formation is negligible compared to the other two reactions. The fluidized bed operates at 510°C and is fed at the same temperature. This temperature should not be exceeded because it promotes carbon formation in the 4^{th} reaction. At 510°C, it may be assumed that 85% of the limiting reactant reacts in the primary reaction, 3%

reacts to form 2-chloropropene, and 12% reacts to form dichloropropene. A minimum of 100% excess propylene is required.

Reaction Section

The PFD for the reaction section is given in Figure 1. The reactants are stored in tanks which are not shown. There are two tanks for each reactant, each holding a one-day supply, one in a filling mode and the other in a feeding mode. The reactants are stored at ambient temperature (which may be assumed to be 25°C) as a vapor/liquid equilibrium mixture, and the feeds to the process are liquids. The feed to the reactor must be at 8 bar and the crude allyl chloride product must be at least 5 bar. The pressure drops across process units are given in Table 1. It may be assumed that pressure drops in pipes beyond Stream 6 are negligible.

Table 1: Pressure Drops across Process Units in Feed Section

Unit	ΔP (bar)
Fired Heater	0.75
Mixing Point	0.40
Reactor	0.50
E-602	0.35
E-603	0.35

The reactor feed must be at 510°C. Heat generated in the reactor is removed by Dowtherm A™, and high-pressure steam is made in E-601. Medium-pressure steam is made in E-602, and Stream 8 should be at 200°C. Since both high-pressure and medium-pressure steam can be used elsewhere in the plant, credit may be taken for its generation. In E-603, the crude allyl chloride product is cooled to 50°C, the required temperature. Stream 8 must contain the required production rate of allyl chloride (plus impurities which will be separated in the separation section).

Refrigeration Section

In the separation section, which will be studied in more detail later, refrigeration is required in one heat exchanger and in three distillation column condensers. Propylene is used as the refrigerant. The propylene refrigeration cycle is illustrated in Figure 2. In E-604, the crude allyl chloride product is cooled to from 50°C to -50°C at approximately 2 bar. In E-606, a mixture of HCl and propylene is condensed at -57°C and 1.4 bar (Q = -1940 MJ/h). In E-611, 0.8 kmol/h of propylene is condensed at -40°C and 1.5 bar. In E-613, 19 kmol/h of 2-chloropropene is condensed at 30°C and 1.4 bar.

For the vessel, V-607, which is a vapor-liquid separator, it should be sized for a 10 minute liquid residence time under the assumption that it contains one-half liquid.

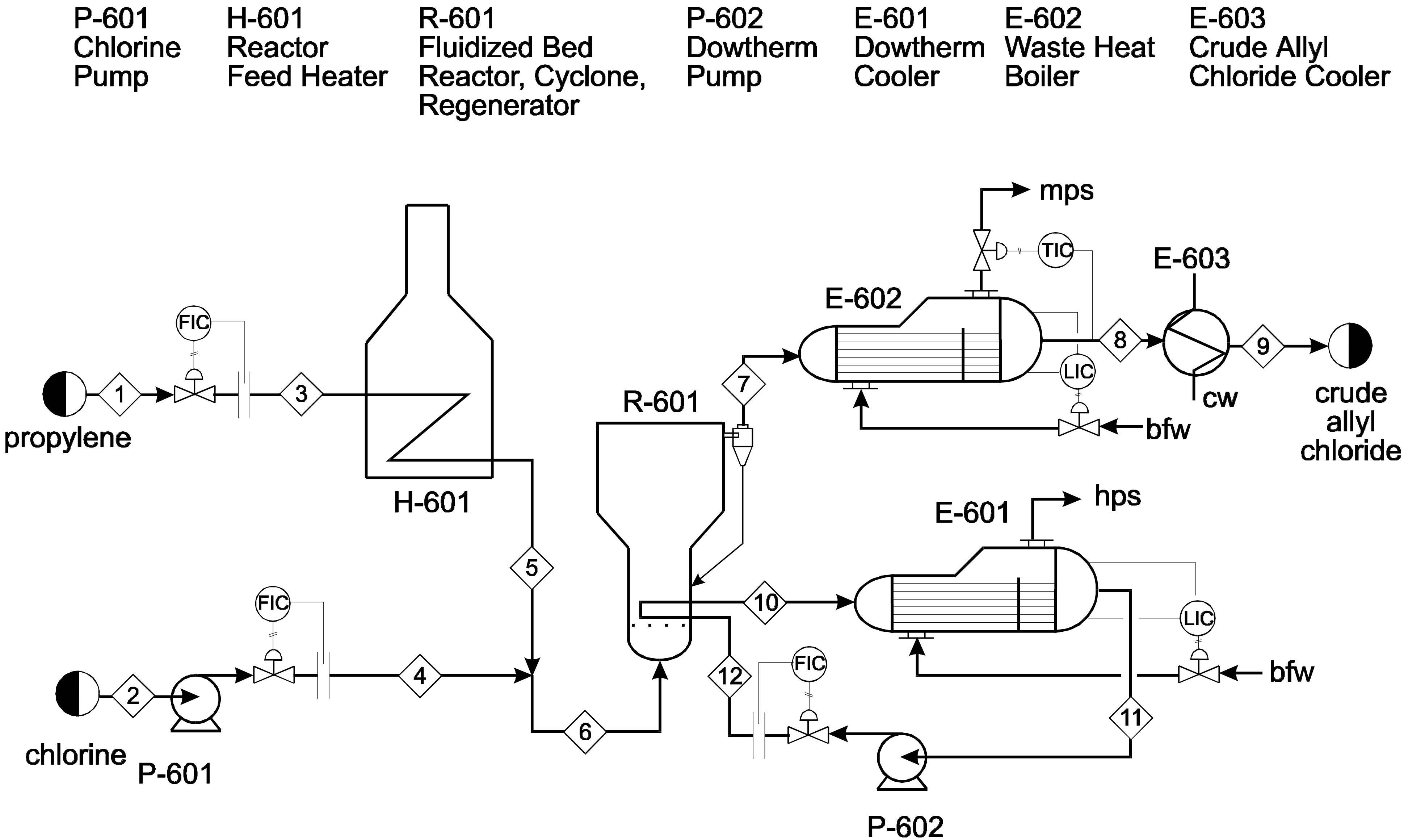


Figure 1: Reaction Section of Allyl Chloride Process

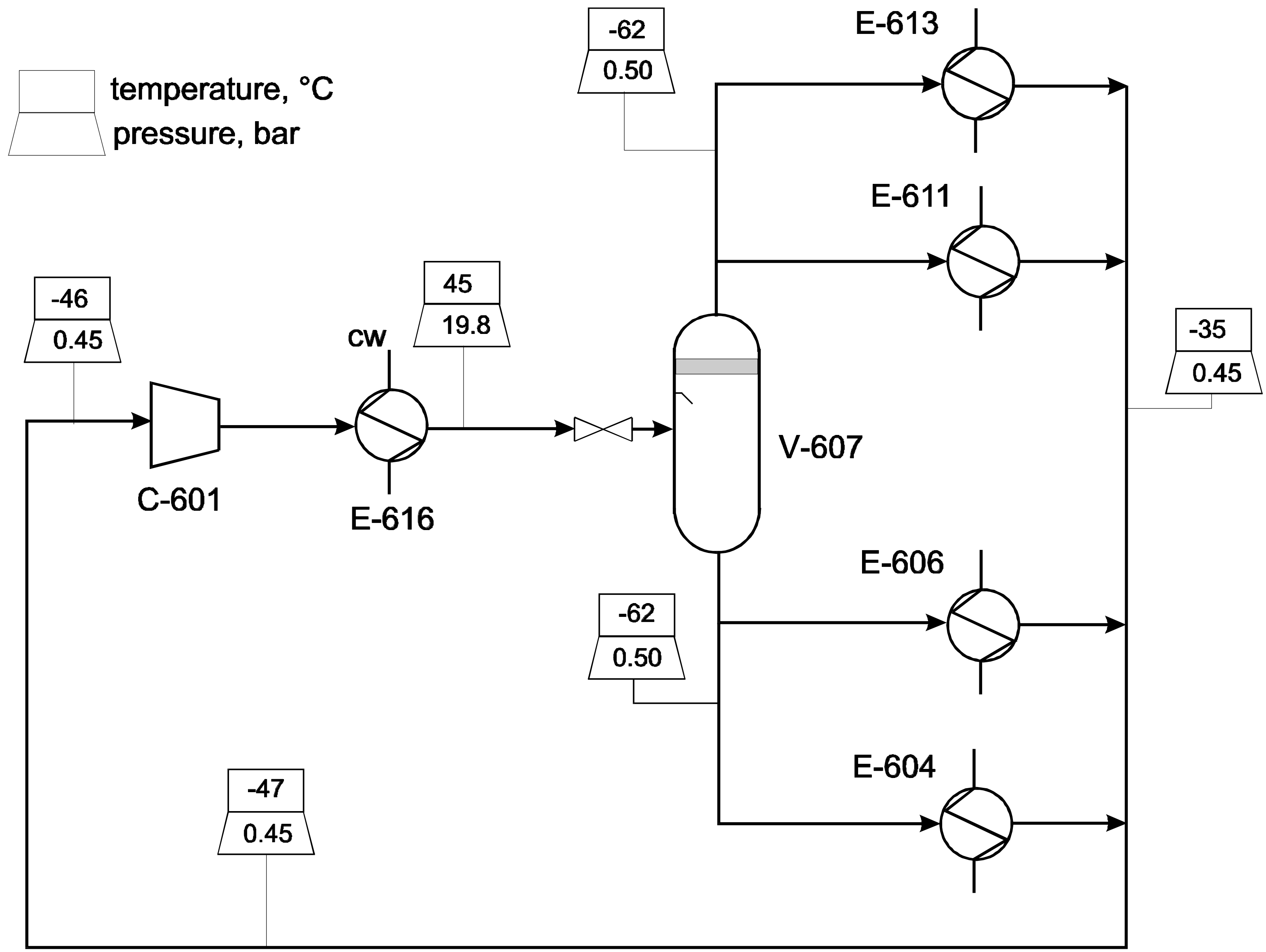


Figure 2: Propylene Refrigeration Loop

Assignment

Your assignment consists of four "mini-designs."

1. **Optimization of the Power Cycle.** (ChE 111 and 142) You are to determine the optimum topology (equipment sequencing) and optimum conditions for the refrigeration loop. The objective function is the Equivalent Annual Operating Cost (EAOC) of refrigeration ($/y). The *EAOC* is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + \text{operating costs for refrigeration loop} \qquad (1)$$

   where *CAP* = the installed cost of equipment in the refrigeration loop and

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \qquad (2)$$

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

2. **Optimization of the Feed Section.** (ChE 110 and 142) Refer to Figure 1. You are to determine the optimum pipe sizes for Streams 1-6. Equivalent pipe lengths can be determined from the attached plot plan (Figure 3). Pipe runs are at 4 m elevation off the ground, and you should add 90° elbows as necessary. The objective function is the *EAOC* (see Eq. (1)) for the piping and pumps (do not include tank costs), where *CAP* includes the cost of pipes and pumps and operating costs include the electricity to run the pumps. You are also to size and cost the feed tanks (1 day of liquid storage required - 2 tanks required for each reactant, one for filling and one for feeding - assume 70% full with liquid) and determine the conditions for propylene and chlorine storage. Both reactants are to be stored as vapor/liquid mixtures and are to be fed to the process as liquids. Specify the elevation of each tank. We have a supply of a feed pumps used in our other plants which we would like to use in this plant, and pump and NPSH curves for these pumps are attached (Figures 4 and 5) We would like the flexibility for 35% scale-up in the future.

3. **Optimization of the Dowtherm AÔ Loop.** (ChE 110 and 111) The heat exchanger and pump should be optimized together. *CAP* should include the cost of the pump and of the heat exchanger. Operating costs should include the cost of pumping and the cost or credit for the heat removal medium in the heat exchanger. We also have a supply of the pump used in our other plants which we would like to use in this plant, and the pump curve is attached (Figure 6). The loop operates above 10 bar, at which pressure the Dowtherm A™ is not volatile below 400°C. The pump and pipes should be sized to allow for 35% scale-up in the future. Equivalent pipe lengths should be determined from the attached

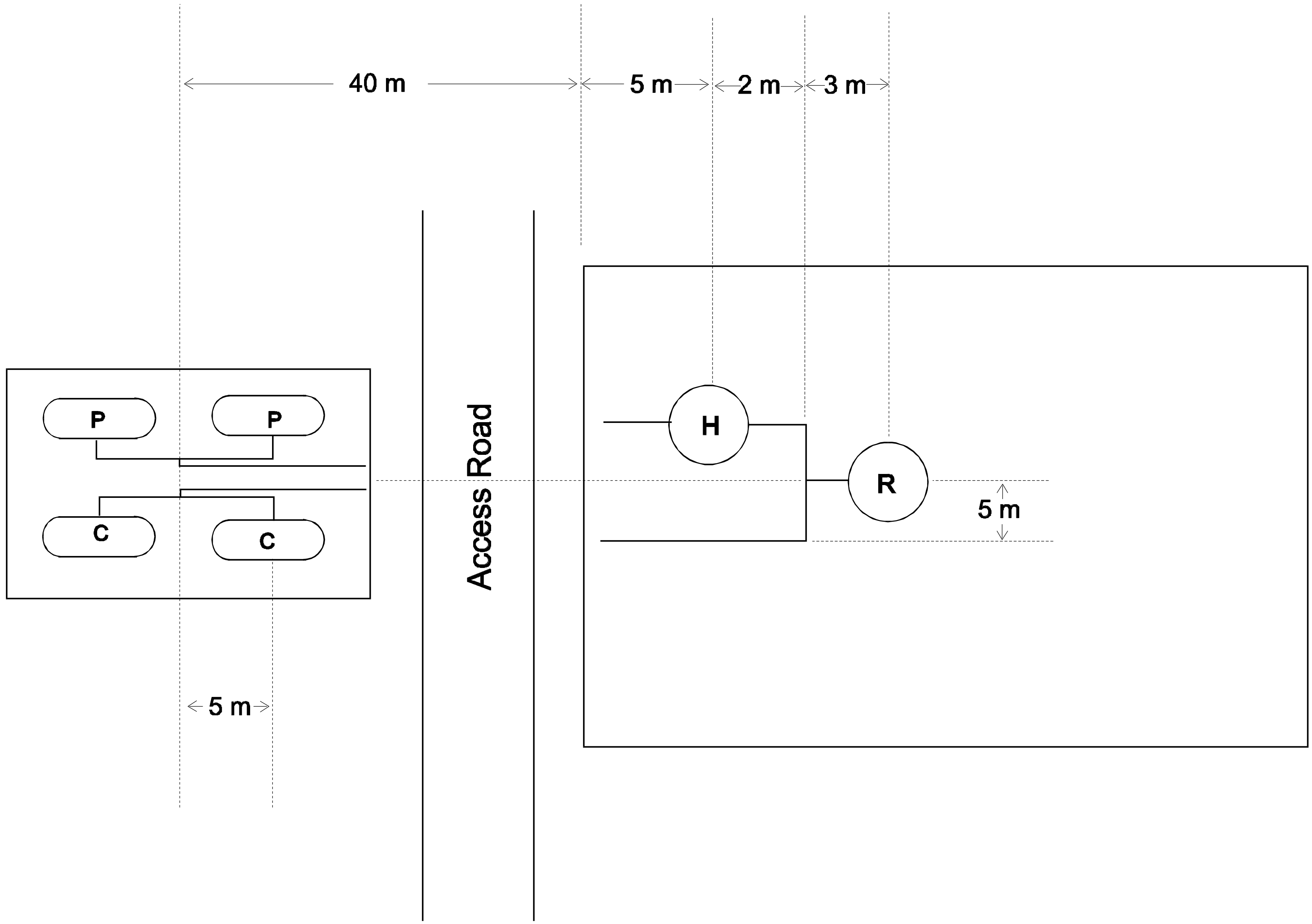


Figure 3: Partial Plot Plan for Allyl Chloride Production Feed Section

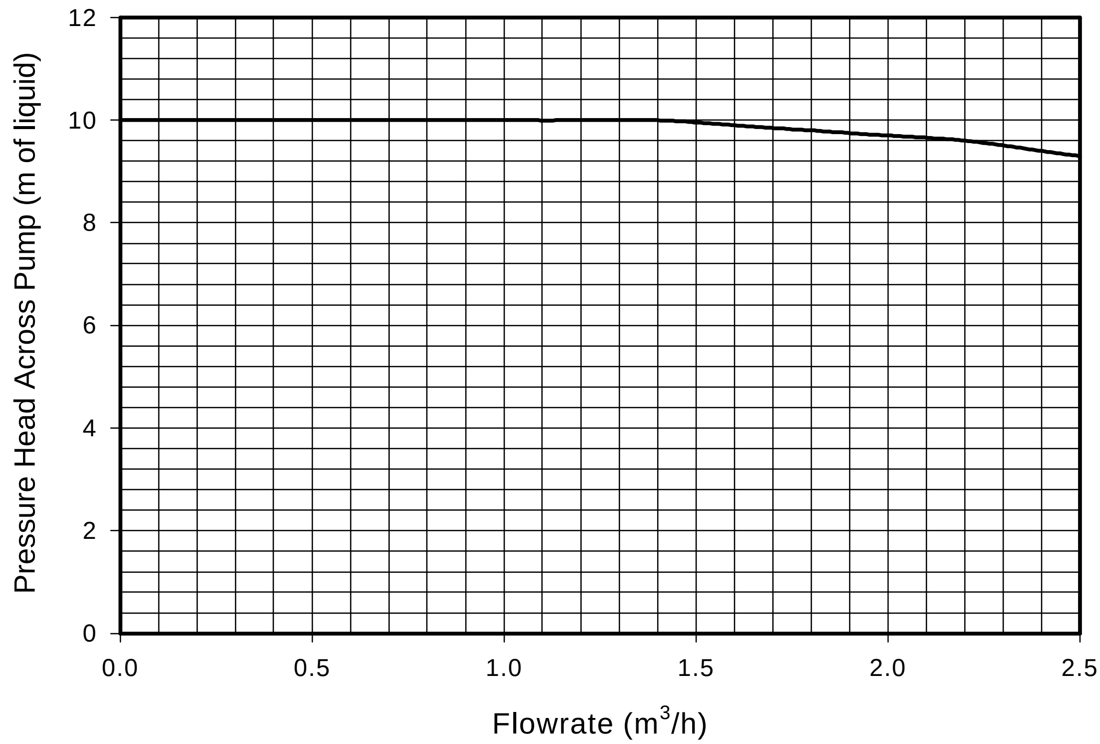


Figure 4: Pump Curve for Feed Pump

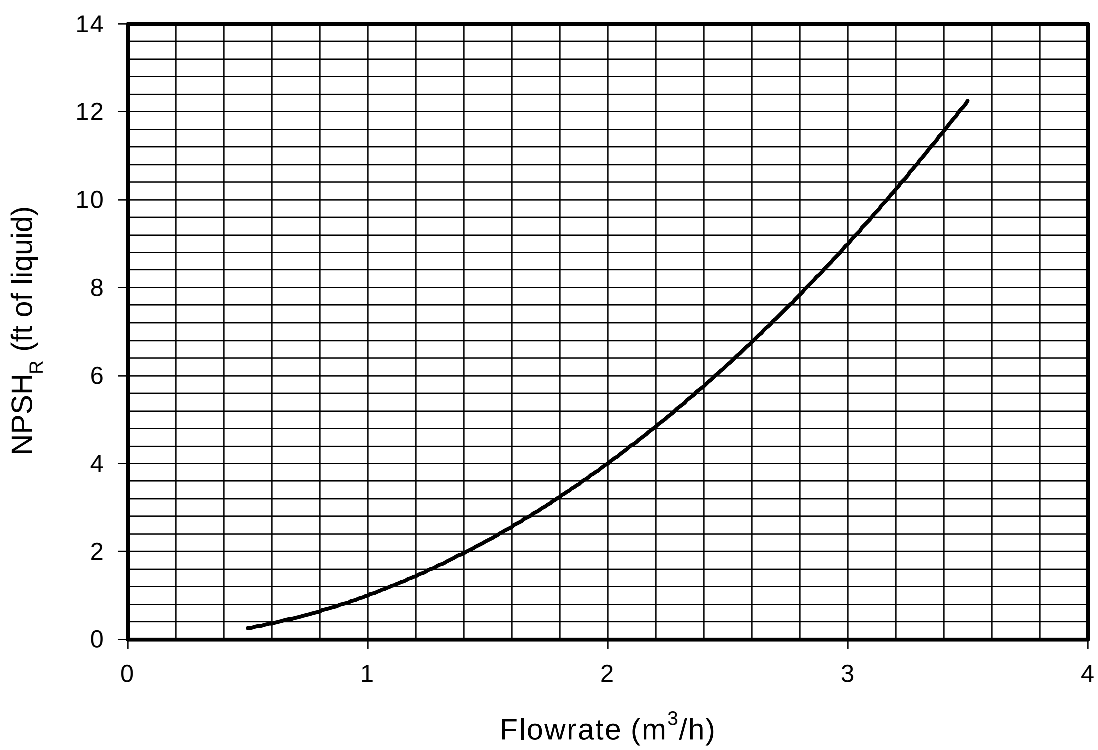


Figure 5: NPSH Curve for Feed Pump

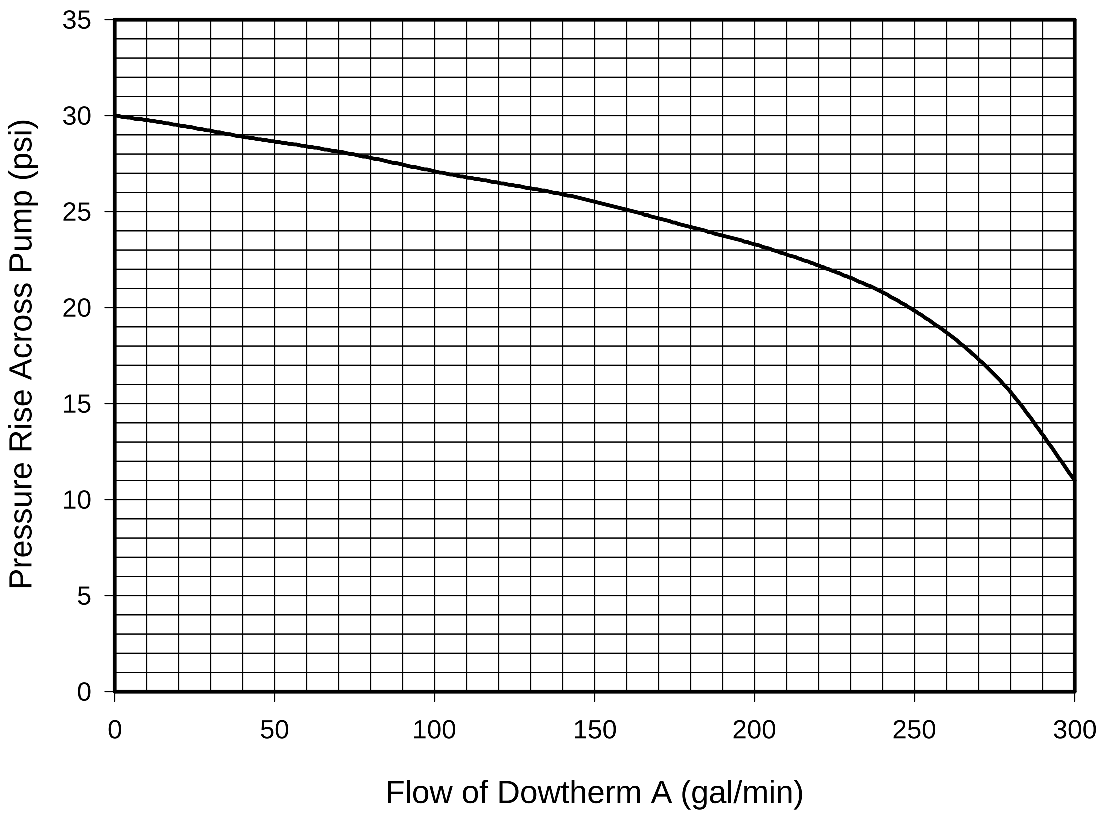


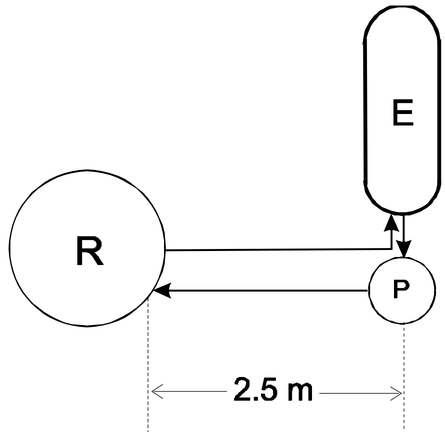
Figure 6: Pump Curve for the Dowtherm A Pump

plot plan (Figure 7). Pipe runs are at 4 m elevation off the ground, and you should add 90° elbows as necessary.

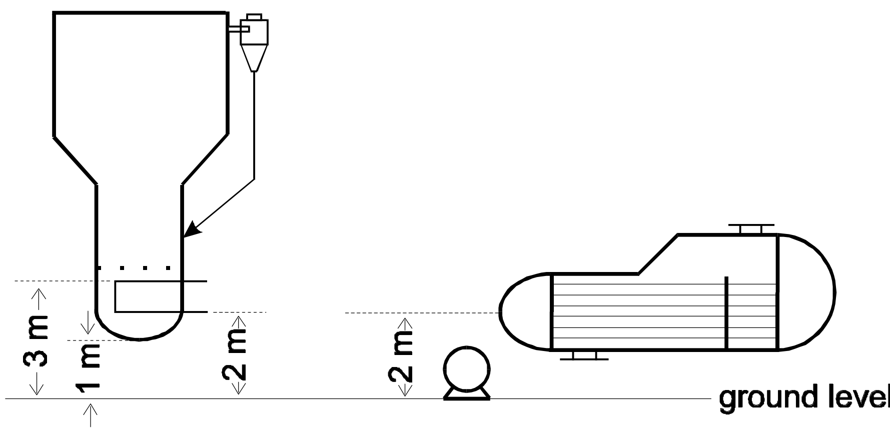
4. **Determination of Break-even Price for Crude Allyl Chloride.** A Chemcad simulation for your best case should be presented. The break-even price (BEP) for crude allyl chloride product should be calculated. The best case is defined as the optimum case for "mini-designs" 1-3, above, plus any other changes to the process that you recommend. The break-even price for crude allyl chloride product is calculated as follows:

$$BEP = \frac{CAP\left(\frac{A}{P}, i, n\right) + \text{cost of reactants} + \text{operating costs} - \text{byproduct revenue}}{\text{kg allyl chloride in crude product}} \tag{3}$$

where *CAP* is the installed capital cost for the entire reaction section. Neglect the cost of pipes in this analysis.



Top View



Side View

Figure 7: Plot Plan for Dowtherm A™ Loop

Cost Data

Raw Materials

Benzene (highest purity)	see *Chemical Marketing Reporter*
Propylene (polymer grade)	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/kW h
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)

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)$^{0.6}$
Compressors	\$770 (power, kW)$^{0.96}$ + 400 (power, kW)$^{0.6}$
Turbine	\$$2.18 \times 10^5$ (power output, MW)$^{0.6}$ assume 65% efficiency
Fired Heater	\$635 (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 $3 < L/D < 20$ P = absolute pressure, bar
Reactor	assume to be \$750,000
Storage Tank	\$1000$V^{0.6}$ 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 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 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:

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 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. The written project report is due by 11:00 a.m. Friday, November 21, 1997. 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 so neatly. Calculations that cannot be easily followed will lose credit.

Since this project involves four “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 “mini-design.” With this organization, there is no need for a separate section 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. A 5-10 minute question-and-answer session will follow. Refer to the document entitled *Oral Reports* for instructions. The oral presentations will be Monday and Tuesday, December 1 and December 2, 1997 from 11:00 a.m. to 1:00 p.m. each day. 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, 111, and ChE 142.

Groups

You may do this projects in a group of three or four. Since there are 23 students doing the project, there will be seven groups. Five groups will have three members and two groups will have five members.

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.