ChE 183 Spring 1997

Major 3: Design and Optimization of a New 20,000 Metric Tons Per Year Facility to Produce Allyl Chloride at La Nueva Cantina, Mexico

17 January 1997
Written Report Due Monday February 17, 1997 at 9:00 a.m.

Background

Recent developments at the Alabama plant have brought into question the stability of our allyl chloride production capacity. It has been noted that the North American market for allyl chloride consumption will probably grow extensively in the next decade and that additional production capacity may be needed. In order to maintain our current market share and to remain competitive in this market, it may become necessary to build a new allyl chloride facility.

With this in mind, a new (grass roots) production facility to produce commercial grade allyl chloride is being investigated. This facility would most likely be situated in La Nueva Cantina, Mexico close to our petrochemical facility which would be able to supply propylene. The supply of chlorine from local manufacturers will also be plentiful. Your group has been given the task of doing a process estimate for this new facility.

Assignment

Your assignment is to design and optimize a new grass roots 20,000 metric tons per year allyl chloride facility. This facility will produce commercial grade allyl chloride from the synthesis reaction between propylene and chlorine. The front end process is to use fluidized bed technology similar to that currently in use in Unit 600 at Beaumont, Texas. This assignment concerns the design of a new plant and, except for the fluidized bed reactor unit, the plant may be reconfigured in any way that you feel is appropriate. For the fluidized bed reactor, kinetic equations are not available, therefore, your design should be similar to the Beaumont unit. With this in mind, the reactor temperature should be close to 510°C with the minimum inlet temperature set at 450°C. The ratio of propylene to chlorine into the reactor should remain the same as currently used. Your final design should be the one which maximizes the net present value (NPV) of the project under the following economic constraints:

After tax internal hurdle rate = 10%
Depreciation = MACRS schedule over 5 years (see Problem 4.18)
Taxation rate = 15% (Mexico)
Labor costs to be based on U.S. equivalent wage rate
Construction period = 2 years
Project plant life = 10 years after start-up

Additional process information and some hints regarding problem solving strategy are given below. The guidelines for written and oral reports given in Chapter 22 should be followed for this assignment. For your recommended (optimized) case, you must include the following items in the main written report:

A PFD for the whole process (Use guidelines in Chapter 1)
A flow table for the optimized process (to include T, P, total mass and mole flows, vapor fraction and component mole flows for each stream)
A table with all purchased equipment costs and pertinent equipment details
A table with all manufacturing costs
A CHEMCAD report for your final optimized case. This output should appear in the appendix along with other pertinent calculations and should be the **ONLY** CHEMCAD output in your report.

For your oral report you should prepare a 15-20 minute formal presentation which will be followed by a 35-40 minute question and answer session. Remember to bring a hard copy of your slides to your presentation. These should be stapled together and ready to give to your audience (only one hard copy is required).

Problem Solving Methodology

The optimization of a process as large and complicated as this one is not a trivial matter. To help you in this endeavor, the following hints are given. (You may use all or none of them as you see fit.) You may also wish to read Chapters 18 and 19.

(1) When running initial case studies using a process simulator, you should use any short-cut methods for simulating distillation columns that are available. Avoid the rigorous methods for this type of preliminary work. You should use the rigorous (tray-to-tray) methods at the end of your work for the optimized case.

(2) Establish a base case from the information provided. This should include operating costs and capital investments for the process shown in Figures 1 and 2, using the new production rate of 20,000 metric tons/year. You should make sure that you have all the equipment and equipment and operating costs included.

(3) See where the major capital investment and major variable operating costs lie, and use this information to focus on where your optimization should begin.

Note: This is a multivariable optimization, and within the time frame given for solving this problem, you can afford to concentrate on only a few variables. Identify the key decision variables to be manipulated, i.e., the variables which have the greatest impact on the NPV.

(4) Do not let the computer turn your mind to mush! Think about how changes in operating variables, etc., affect the economics and try to predict the direction in which the NPV will

change as each variable changes. You should be able to rationalize, at least qualitatively, why a certain change in a variable causes the observed change in the NPV.

Process Information

To help you in this task, the following information has been included with this assignment.

(1) A flowsheet and a process description for the existing Unit 600 are included in Figures 1 and 2 and Tables 1 and 2.

(2) Product specifications are included in Table 3.

(3) Note that the current process (Unit 600) is very energy intensive, since very cold temperatures and expensive refrigeration are used throughout the process. Remember that the existing Beaumont plant was designed over thirty years ago when electricity and energy were relatively cheap. The optimal process configuration for today's conditions may be significantly different from that of the existing facility!

(4) CHEMCAD™ Simulations are included and can be accessed on the ChE 182 directory of the LAB directory on G: drive by typing MAJOR3 which will copy all the CHEMCAD™ files to a floppy disk. These flowsheets represent the simulation of the current allyl chloride facility in Beaumont, TX. The flows and compositions are those at design conditions and are the same as shown on Figures 1 and 2 of this assignment.

The simulation named **ALLYL2** is for the PFD shown in Figure 1. The simulation named **REFRIG** is the simulation for the refrigeration loop shown in Figure 2. Clearly the costs of both these processes and the front end of the process (given in Majors 1 and 2) must be used to estimate the capital and operating costs of the plant. Note that the new facility has approximately twice the throughput of the Beaumont Facility at design conditions.

IMPORTANT

Thermodynamics: The SRK thermodynamics package should be used for the enthalpy and K value options for the entire process **EXCEPT** for any unit in which HCl vapor is condensed in the presence of water, e.g., T-602. Due to the fact that HCl ionizes in water, the standard thermodynamic models do not work well. For this special case, you **MUST** use the PPAQ option for K value model and the heats of solution option for the enthalpy model. This has already been programmed in the simulation for Figure 1 (ALLYL2) by using these local models for the absorber unit. It is your responsibility to ensure that this option is used for the HCl separator (and any other unit in which V-L equilibrium between HCl and Water is required) in you simulation.

You may assume that tray efficiencies are the same as for the Beaumont Facility (i.e., compare the CHEMCAD output to Figure 1 to get the efficiency). For the HCl absorber, assume that each theoretical plate requires 4 ft of packing. The HCl traps (V-603A/B) contain a heat transfer surface to condense water vapor and a packed bed of absorbent to adsorb the remaining water and traces of HCl and other organics. This pair of condensers/adsorbers operates continuously with one unit on and one on stand-by. The superficial gas velocity through these vessels should not exceed 2 m/s. For other design parameters, use the guidelines given in Chapter 9.

Table 1: Flow Summary Table for Allyl Production Process, Figures 1 and 2

Stream No.	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	50	-50	-50	45	-57	-57	25	54	63	45
Pressure (bar)	2.09	1.50	1.50	1.50	1.40	1.5	3.0	1.2	1.2	20.0
Vapor Fraction	1.0	1.0	0.0	0.0	0.0	0.087	0.0	0.0	1.0	0.0
Molar Flowrate (kmol/h)										
Propylene	58.08	2.69	55.39	0.55	3.69	57.53	-	0.14	57.39	57.94
Allyl Chloride	15.56	0.01	15.55	15.54	-	0.02	--	-	0.02	-
2-chloro propene	0.46	-	0.46	0.46	-	-	-	-	-	-
dichloro propene	1.81	-	1.81	1.81	-	-	-	-	-	-
hydrogen chloride	19.70	4.15	15.55	-	1.04	19.70	-	19.70	-	-
water	-	-	-	-	-	-	99.30	86.26	13.04	-
Total Molar Flowrate (kmol/h)	95.61	6.85	88.76	18.36	4.73	77.25	99.30	106.10	70.45	57.94

Stream No.	15	16	17	18	19	20	21	22	23	24
Temperature (°C)	-40	59	60	30	30	103	55	55	40	-46
Pressure (bar)	1.5	2.0	1.5	1.4	1.4	1.5	1.4	1.4	1.1	0.5
Vapor Fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Molar Flowrate (kmol/h)										
Propylene	0.80	-	-	0.21	-	-		-	-	602.5
Allyl Chloride	0.01	15.53	15.52	0.66	0.02	0.08	6.92	15.44	-	-
2-chloro propene	-	0.45	-	18.96	0.45	-	-	-	-	-
dichloro propene	-	1.81	1.81	-	-	1.80	-	0.01	-	-
hydrogen chloride	-	-	-	-	-	-	-	-	-	-
water	-	-	-	-	-	-	-	-	8.86	-
Total Molar Flowrate (kmol/h)	0.81	17.79	17.33	19.83	0.47	1.88	6.92	15.45	8.86	602.5

Table 2: Process Description of Unit 600

Refer to the process flow diagram for Unit 600, Allyl Chloride Purification Process, Beaumont, Texas (Figure 1).

Crude allyl chloride, Stream 5, from the reaction section of Unit 600 (Figure 1 Major 1) enters the Allyl Product Cooler, E-604, at 50°C and 2.1 bar. This stream is cooled to -50°C using the circulating liquid propylene refrigerant. The two-phase mixture leaving E-604 is fed to V-601 where the liquid stream is taken off and is fed to the HCl column T-601. The HCl column removes essentially all the HCl and propylene from the cooled crude allyl chloride feed as overhead product at approximately -57°C. This stream is mixed with the vapor coming from V-601 and is fed to E-607 where it is vaporized with low pressure steam.

The bottom product from T-601 contains essentially all the chlorinated hydrocarbon derivatives and a small amount of propylene. This stream is fed to T-603 where the remaining propylene is removed as the overhead product at approximately -40°C. The bottoms product from T-603 is fed to column T-604 where 95 mole % 2-chloro-propene is removed overhead at approximately 30°C. The bottom product from T-604 is fed to the allyl tower, T-605, where 99.9% by mole pure allyl chloride is removed as overhead product at 55°C and the sent to storage. The bottom product from T-605 contains >95 mole % 1,2,dichloro-propene and this stream is sent to storage after being cooled in an off-site heat exchanger (not shown on Figure 1).

The stream leaving E-607 is fed to T-602 where it mixes with water at 25°C. The flow of water is controlled to give an aqueous solution of hydrochloric acid with 31.5 wt % HCl (called 20° Baumé). The vapor stream leaving T-602 contains all the propylene and small amounts of water and HCl. This stream is sent to one of a pair of acid traps, V-603 A&B, where the water and HCl are removed (by condensation and adsorption onto activated carbon and other sorbents). The vapor stream leaving the absorbers is essentially pure propylene. This propylene stream is sent to a two stage compressor C-601 A&B with intercooler E-408 and condenser E-409. The stream leaving the condenser is a liquid at 45°C and is recycled to the propylene storage tank for Unit 600.

Four of the exchangers in Unit 600 (E-604, E-606, E-611 and E-613) require heat to be removed from the process stream at temperatures below 35°C. In order to do this a refrigeration system is required. In Unit 600, this is achieved by circulating a stream of cold (-62°C) propylene through these exchangers. The refrigeration loop is shown in the second PFD for Unit 600, Figure 2. The refrigeration is achieved by taking a high pressure (20 bar) stream of liquid propylene (45°C) and flashing it down to low pressure (0.5 bar). Cooled liquid and vapor propylene streams (-62°C) are sent to the four process exchangers where they provide the necessary cooling. The warmed propylene vapor (-47°C) is recycled back to the refrigeration loop compressors, C-602 A&B, the intercooler, E-616, and the condenser, E-617. A make-up propylene stream is provided to account for minor system leaks.

Table 3: Feed and Product Specifications and Byproduct Costs (Unit 600)

Feed	**Supply Condition**	
Propylene	Saturated Liquid at 25°C	
Chlorine	Saturated Liquid at 25°C	
Deionized Water	25°C, 3 bar	
Product	**Required Purity**	**Battery Limit Condition**
Allyl Chloride	> 99.9% by mole allyl chloride	Liq, T < 55°C, P >1.4 bar
Byproduct	**Required Purity**	**Battery Limit Condition**
Mixed Chlorides	> 95% by mole 1,2 dichloro-propene.	Liq, T < 50°C, P >1.2 bar
2-chloro-propene	> 95% by mole 2-chloro-propene	Liq, T < 50°C, P >1.2 bar
20° Baumé Hydrochloric Acid	31.5% by weight HCl ±0.1 wt %	Liq, T < 25°C, P >1.2 bar

Byproduct	**Selling Price**
mixed chlorides	$ 0.10 /kg+
2-chloro-propene	$ 0.10 /kg+
20° Baumé HCl	From *Chemical Marketing Reporter*

+These are credits that we will receive from our petrochemical complex for supplying these chemicals which must meet the specifications given above. We may alternatively pay to dispose of these chemicals at a cost of $0.10 /kg. For this case, no specifications need to be met (i.e., these streams are now waste streams rather than byproducts).

Waste Stream	**Cost of Disposal**
Spent Absorbent	$ 0.20 /kg of HCl + water + hydrocarbons collected on sorbent
Waste Water	tertiary treatment, see Chapter 3

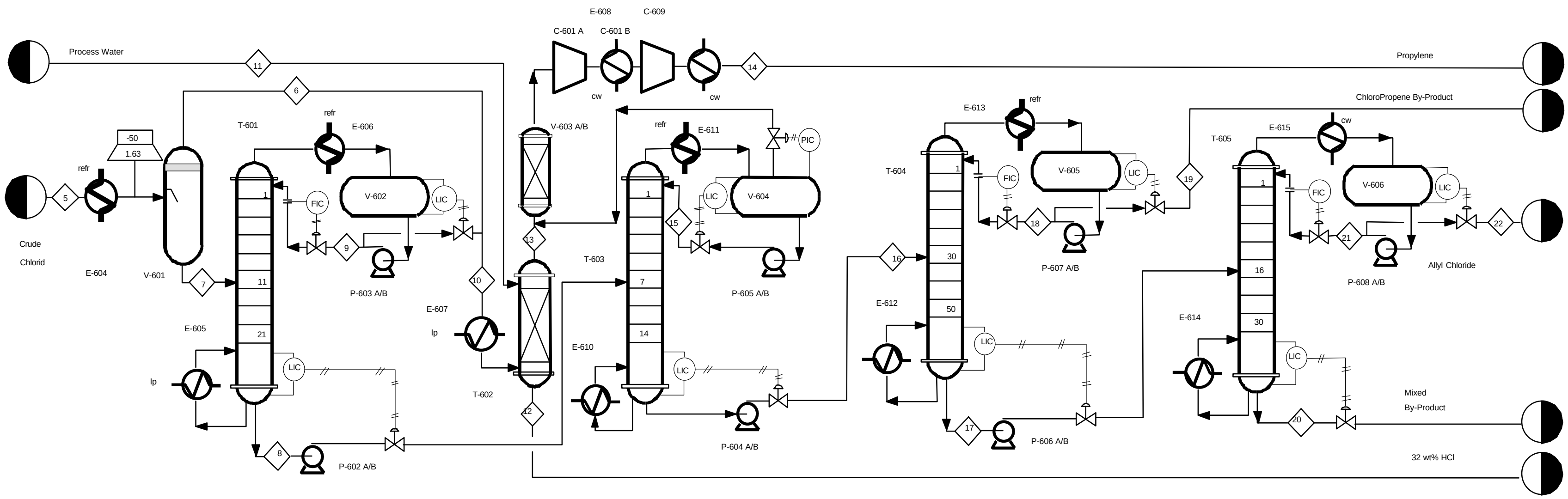

Figure 1: Separations Section of Allyl Chloride Production Facility (Unit 600)

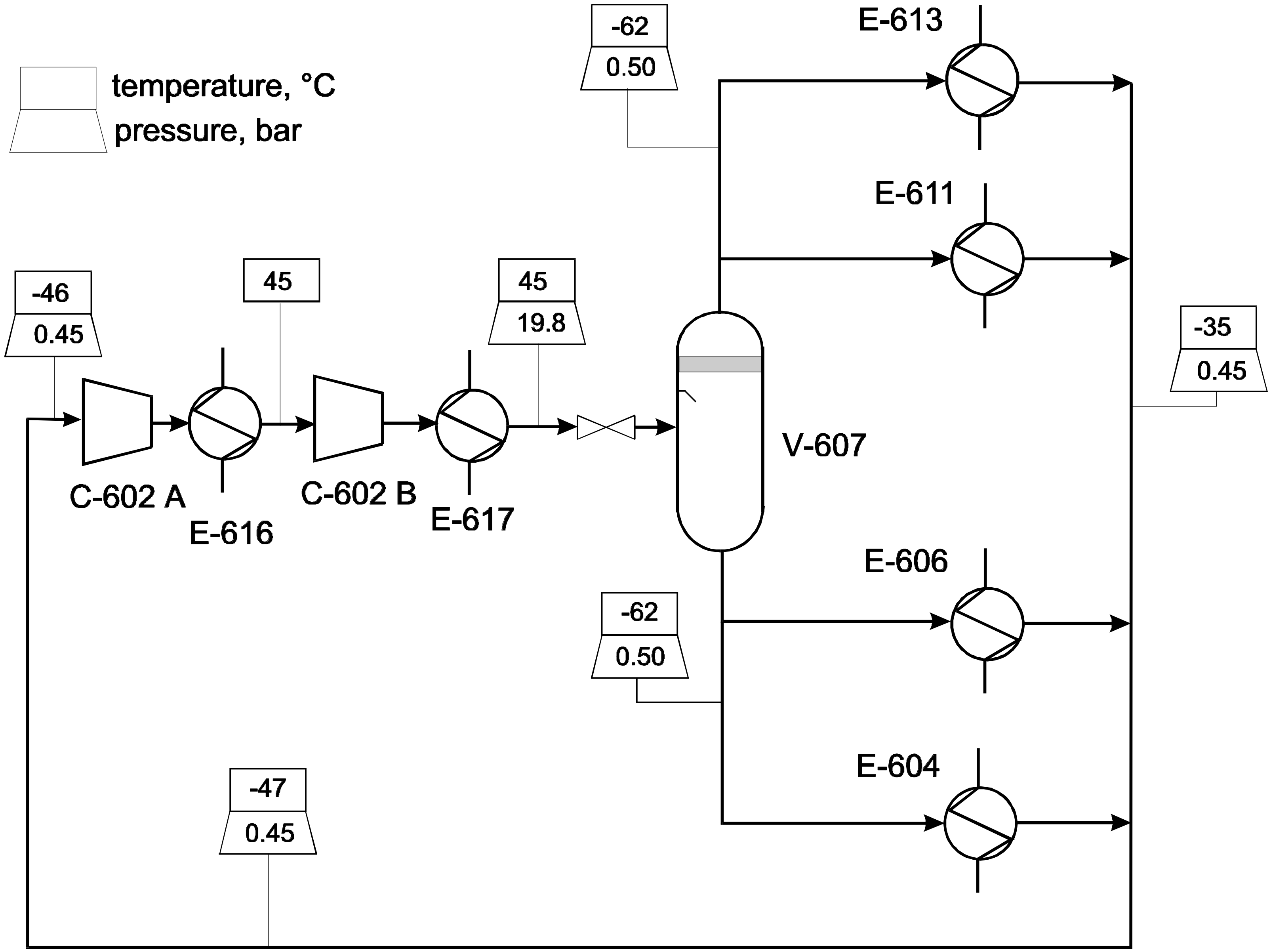

Figure 2: Propylene Refrigeration Loop