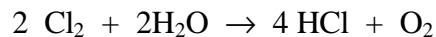


Material Balances Project: Allyl Chloride Manufacture

We plan to evaluate the economics for a process to manufacture allyl chloride from propylene and chlorine. The pertinent reactions, selling prices for reactants and products, and a rough flow sheet are included on the following pages.

You are expected to form small groups and to evaluate the process to determine operating conditions that will produce a maximum profit for a plant that produces 10,000,000 kg/year. No information has been provided about operating costs, so that you should consider profit to be the difference between product value and feedstock cost.

On examining the attachment, I noticed two items. The first is that there must be an optimum reaction temperature that will maximize profits. The second is that unreacted chlorine has not been accounted for. There are two possible treatments of unreacted chlorine that you should consider. The first is recycling the unreacted Cl₂ from the separation section, back to be mixed with fresh feed. The second option is to convert unreacted chlorine in the separation section to HCl and O₂. The HCl would be sold as 32wt% hydrochloric acid and the oxygen would be vented to the air. The reaction for converting chlorine to hydrogen chloride is listed below:



Problem:

You, as a new process engineer, are asked to calculate the most profitable mode to operate an allyl chloride production unit. You are to determine the operating temperature and how the unreacted Cl₂ should be handled. There are a large number of cases that need to be evaluated. You should calculate the profit (loss) for each case and provide stream tables for each case.

You may not use CAD software, but you may use a spreadsheet to do calculations or you may write your own program. You may use the VAX or a PC. Any programming language is acceptable. However, if you write a program, you should check your results for several cases with hand calculations to confirm that the program was written correctly.

Group Formation

A group is to consist of at least 3 and no more than 4 members. No other combinations are acceptable. You are free to make groups by yourselves. When you have formed a group, please write the names of its members on the chart posted on Dr. Kugler's office door. Individuals who do not form their own groups will be assigned to one.

Reports

Each group will be expected to prepare a written report recommending a best operating condition, and comparing the recommended condition to all you have considered. The report should follow the department's design report format. Data should be in the form of graphs and tables since this serves to both condense the results and make them easily understandable. The appendix should include stream tables on all cases considered, a statement on your calculation strategy, the algorithm used, a hand calculation for one case, and a copy of your computer program.

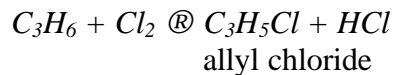
Report Authors

Although work on a group report can never be divided equally, only those members of the group making substantial contributions to the final report should be listed as authors.

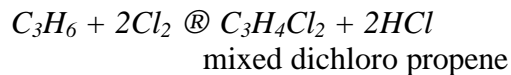
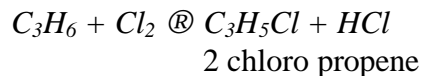
E.L. Kugler
October 28, 1996

Project Background - 1996/97

Main reaction



Side reactions



Selectivity as a function of temperature

Temperature	Selectivity allyl/everything	2 chloro/di chloro	Single pass conversion
440	13.22	0.489	55%
460	10.49	0.389	70%
480	8.43	0.312	82%
500	6.85	0.253	92%
520	5.62	0.208	99%

selling price of 99.5 wt% pure allyl chloride = \$1.72/kg

selling price of 32wt% hydrochloric acid = \$0.075/kg

waste disposal costs of 2 chloro propene = \$0.20/kg

waste disposal costs of di chloro propene = \$0.20/kg

cost of deionized water = \$0.30/1000kg

cost of propylene = \$0.47/kg

cost of chlorine = \$0.18/kg

ratio of propylene/chlorine at reactor inlet = 5:1 (by mole)

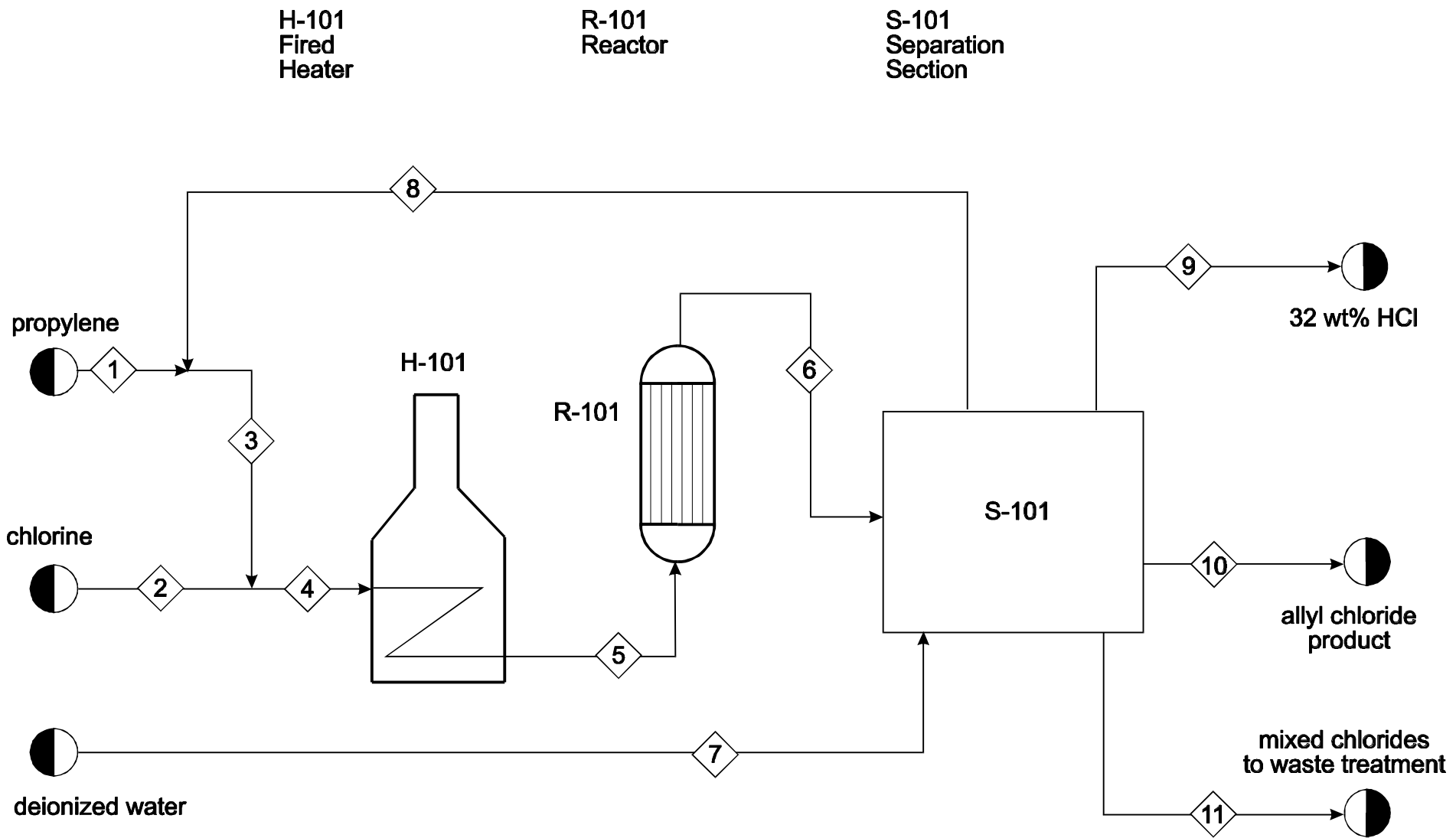
Separation Factors

Assume that 99% of the allyl chloride is recovered as product and remaining 1% goes to waste treatment.

Assume that the remainder of the allyl chloride product contains only 2 chloropropene.

Assume that all dichloropropene and the remainder of the 2 chloropropene goes to waste treatment.

Assume that all the HCl is recovered as 32wt% hydrochloric acid and sold for profit.
Assume that all the deionized water is used to make the 32wt% hydrochloric acid, i.e., only buy the correct amount to make the acid product.
Assume that all the propylene leaving the reaction section is recovered and recycled.



The Production of Allyl Chloride