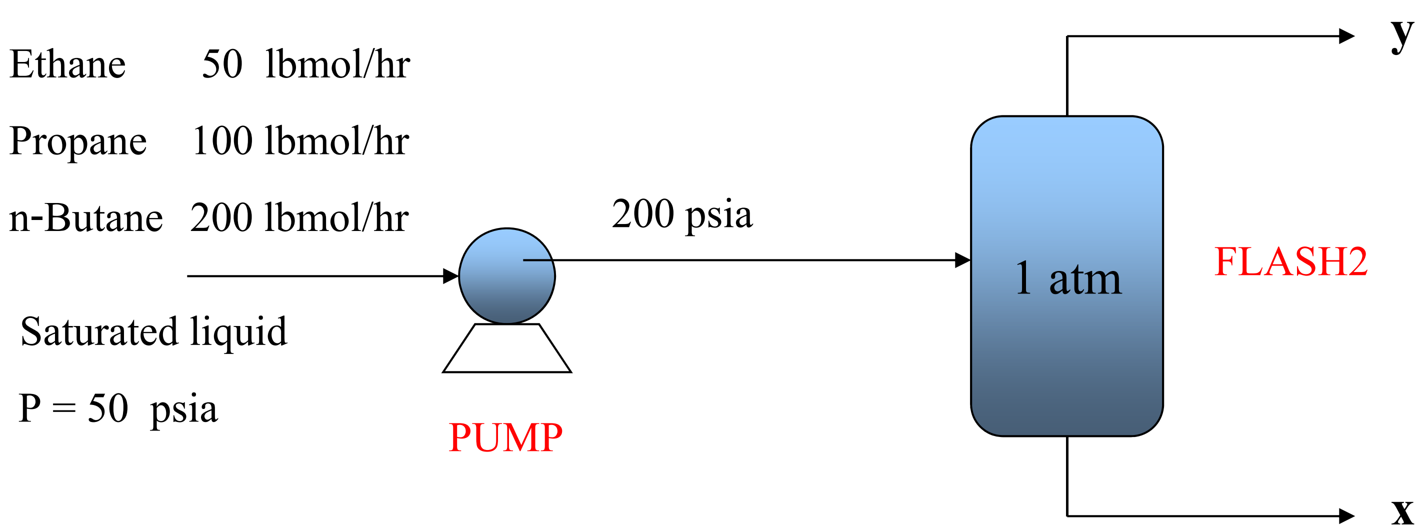
Process Simulation with ASPEN PLUS

CHE654 Course Notes

Section 9: Workshops

These course materials are applicable to Version 8.4 of ASPEN PLUS

Workshop 1: Flashing of Light Hydrocarbons



Use the Redlich-Kwong-Soave equation of state

for property calculations

Workshop Problem 1 (Cont'd)

Answer the following questions:

1. Required pump power input = _______________ hp
2. Feed stream temperature = _______________ ^{o} F
3. Flash outlet temperature = _______________ ^{o} F
4. Vapor fraction in flash = _______________
5. Vapor composition from flash (mole fractions):

6. Liquid composition from flash (mole fractions):

Workshop: Vinyl Chloride Monomer Production

Vinyl chloride monomer (VCM) is produced through a high-pressure, non-catalytic process involving the pyrolysis of 1,2-dichloroethane (EDC) according to the following reaction:

$$C_2H_4Cl_2 \text{ ------> } C_2H_3Cl + HCl \qquad (1)$$

The process flow diagram is shown in Figure 1. The cracking of EDC occurs at 900 ^{o}F and 390 psia in a direct-fired furnace. The pure EDC feed enters the furnace after going through a pump in which its pressure is raised from 120 psia (and 100 ^{o}F) to 390 psia, with a rate of 2000 lbmol/hr.

Vinyl Chloride Monomer Production (Cont'd)

By-products of pyrolysis consist principally of acetylene and chloroprene through the following reactions:

$$C_2H_4Cl_2 \text{ ------> } C_2H_2 + 2HCl \qquad (2)$$

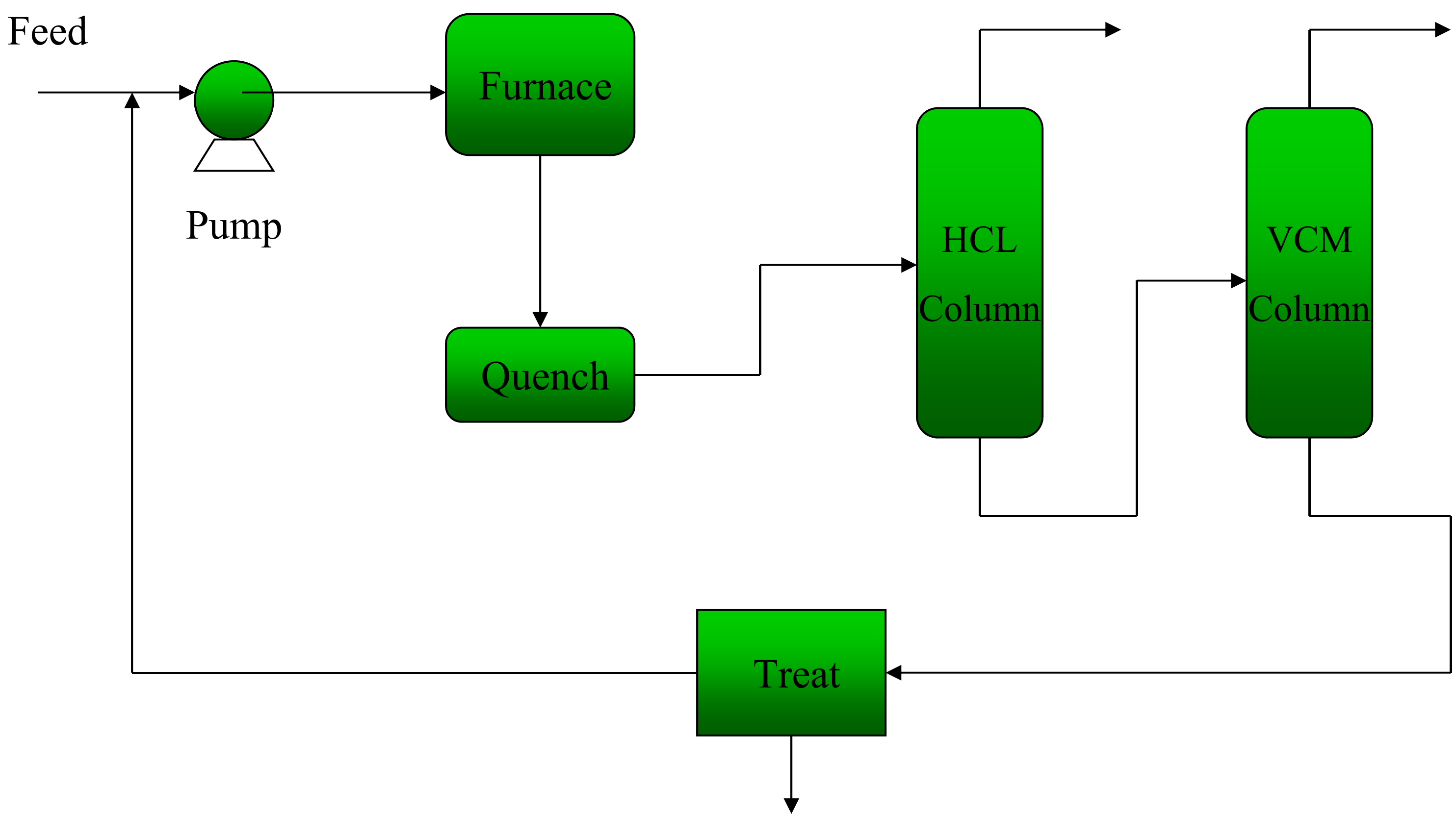
$$C_2H_3Cl + C_2H_2 \text{ ------> } C_4H_5Cl \qquad (3)$$

The overall EDC conversion is maintained at 55%, with a selectivity of 98% for VCM production (reaction 1), and 2% for acetylene (reaction 2). Seventy-five percent (75%) of the acetylene produced is converted into chloroprene.

Vinyl Chloride Monomer Production (Cont'd)

The hot gas from the furnace is quenched to 10 degrees below saturation prior to fractionation. Two distillation column are used for the purification of VCM product. In the first column, HCl is removed overhead and sent to the oxychlorination unit, while at the same time, it is desirable to maintain a target of 50 ppm (by weight) HCL in the bottoms of this column. In the second column, VCM product is delivered overhead, while the bottom stream containing unreacted EDC is recycled back to the cracker. The recycle EDC stream is treated to remove chloroprene which could hinder pyrolysis and fractionation.

Figure 1: Vinyl Chloride Monomer Production Process



Workshop 2: VCM Base-Case Flowsheet Simulation

Develop a base-case ASPEN PLUS simulation for the VCM flowsheet, using the following information:

a) Model the cracker furnace with the RSTOIC reactor model. Consider only the main VCM reaction at this point.

b) Model the reactor effluent quench using an appropriate ASPEN PLUS model. Assume 10 degrees subcooling, and a pressure drop of 5 psia across the quench.

c) Model both the HCL and VCM columns using the DSTWU shortcut model. Specifications for the 2 columns are:

VCM Workshop 2 (Cont'd):

HCL Column:

Theoretical stages	15
Condenser (total) pressure	360 psia
Reboiler pressure	370 psia
HCL recovery in overheads	99.9%
VCM recovery in bottoms	99.9%

VCM Column:

Theoretical stages	10
Condenser (total) pressure	115 psia
Reboiler pressure	120 psia
VCM recovery in overheads	99.9%
EDC recovery in bottoms	99.9%

VCM Workshop 2 (Cont'd):

d) Assume the flowrate of recycle EDC is 1600 lbmol/hr, but do not close the recycle loop from the VCM column. Ignore the treatment block at this point.

e) Use the Redlich-Kwong-Soave equation of state to represent the physical properties of the system.

Answer the following questions:

1. Furnace heat duty = ________________ Btu/hr
2. Quench cooling duty = ________________ Btu/hr
3. Quench outlet temperature = ________________ ^{o}F

VCM Workshop 2 (Cont'd):

4. Did we achieve the 50 ppm target of HCl at the bottom of the HCl column? ___________

   If not, HCl conc. at the bottom of column = _________ ppm (mass)

5. VCM purity in the overhead of VCM column = __________ mole%

6. HCL column key results:

   - Actual reflux ratio = ___________
   - Feed tray location = ___________
   - Top temperature and bottom temperature = _______________ ^{o}F
   - Condenser and reboiler duties = ________________________ Btu/hr

VCM Workshop 2 (Cont'd):

7. VCM column key results:

- Actual reflux ratio = ___________
- Feed tray location = ___________
- Top temperature and bottom temperature = _____________ ^oF
- Condenser and reboiler duties = ___________________ Btu/hr

Workshop 3: VCM Sensitivity and Design-Specs

A) Sensitivity Analysis:

During operation, EDC conversion in the cracker may vary between 50% and 60%. Use the sensitivity analysis capability in ASPEN PLUS to develop plots of furnace heat duty and quench cooling duty as a function of EDC conversion.

B) Design Specifications:

The specified HCL recovery of 99.9% for the HCL column is not sufficient to meet the specification of 50 ppm HCL in the bottoms.

Workshop 3: VCM Design-Specs (Cont'd)

B) Design Specifications (Cont'd):

Use the design-spec capability in ASPEN PLUS to determine the HCL recovery that corresponds to 50 ppm HCL (by weight) in the bottoms from the HCL column.

What is the required HCl recovery in the HCL column in order to achieve the 50 ppm target? _______________

Workshop 4: Introducing a Non-Databank Component

For this workshop, let's assume that chloroprene, a by-product of the EDC cracking reaction, does not appear in the ASPEN PLUS pure component databanks (in reality, it does). However, the following property data are available for chloroprene:

Molecular weight:	88.5364
Critical temperature:	525.0 K
Critical pressure:	42.04 atm
Critical volume:	0.273 m^3/kmol
Critical compressibility factor	0.266
Pitzer acentric factor:	0.19743
Normal boiling point:	59.4 ^oC

Workshop 4 (Cont'd)

Ideal gas heat of formation: 73,010 kJ/kmol

Ideal gas free energy of formation: 114,800 kJ/kmol

Heat of vaporization at T_B: 27,883 kJ/kmol

Ideal gas heat capacity:

$$C_{PIG} = 21.2655 + 0.05355T - 8.0776 \times 10^{-5}T^2 + 1.01287 \times 10^{-7}T^3$$

where C_{PIG} is in Btu/lbmol-R and T is in C.

Workshop 4 (Cont'd)

Vapor pressure:

T(^{o}C)	P(mmHg)	T(^{o}C)	P(mmHg)
0	72.74	80	1391.72
20	181.52	100	2331.65
40	395.67	130	4558.41
59.4	760.27	160	8092.34

Workshop 4 (Cont'd)

Introduce chloroprene into the VCM simulation. Enter the required physical property data using the appropriate GUI forms. Be sure to leave the Component Name column in the Selection tab of the Components Specifications form blank to indicate that chloroprene is a non-databank component.

Use the flowsheet in Workshop 3B as the starting point.

Note: You are given more property data than needed. What are the redundant property data? ____________________________________

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Workshop 4 (Cont'd)

Answer the following questions:

1. Furnace heat duty (for 3 reactions) = ____________________ Btu/hr

2. Quench cooling duty = ____________________ Btu/hr

3. Chloroprene mole flow and mass fraction at the bottom of VCM column

   = ____________________________

4. HCL column parameters:

   – Reflux ratio = __________

   – Distillate to feed ratio = _____________

   – Feed tray location ____________

Workshop 5: RADFRAC Distillation Model

Model the HCL column rigorously using the RADFRAC distillation model in ASPEN PLUS. Using the feed location and the distillate to feed ratio determined from the shortcut calculations of Workshop 4, determine the reflux ratio, condenser, and reboiler duties that will give 50 ppm of HCL in the bottoms of the first column.

Answer the following questions:

1. Calculated reflux ratio = ________________

2. RADFRAC condenser duty = ________________ Btu/hr

3. RADFRAC reboiler duty = ________________ Btu/hr

Workshop 6: Recycle Convergence

Using the VCM flowsheet model prepared in Workshop 4, incorporate the recycle of unreacted EDC to the pump. Before the EDC-rich bottoms stream from the VCM column is fed into the pump and then to the furnace, it must be treated to remove the chloroprene. Assume that the chloroprene treatment section has a removal efficiency of 95%, and that the outlet streams from the treatment block are saturated liquid at 120 psia (bottom pressure of the VCM column).

Workshop 6: Recycle Convergence (Cont’d)

Using the EDC recycle to the pump as the tear stream, compare the following convergence strategies:

a) Nest the HCL bottoms purity design-spec for the HCL column inside of the recycle convergence.

b) Converge the design-spec and recycle stream simultaneously.

Which strategy converged faster in this model? ____________________

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