PRODUCTION OF ALLYL CHLORIDE

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Introduction:

Allyl chloride is produced by the thermal chlorination of propylene at elevated temperatures and relatively low pressures. Allyl chloride is used as a precursor in the production of allyl alcohol, glycerin, and a variety of other products used in the pharmaceutical industry.

Reactions:

Main Reaction:

$C_3H_6 + Cl_2 \longrightarrow C_3H_5Cl + HCl$ $\quad \Delta H_{298K} = -112KJ/mole$

Allyl Chloride

Side Reactions:

$C_3H_6 + Cl_2 \longrightarrow C_3H_5Cl + HCl$ $\quad \Delta H_{298K} = -121KJ/mole$

2-Chloropropene

$C_3H_6 + 2Cl_2 \longrightarrow C_3H_4Cl_2 + 2HCl$ $\quad \Delta H_{298K} = -222KJ/mole$

Dichloropropene

$C_3H_6 + 3Cl_2 \longrightarrow 3C + 6HCl$ $\quad \Delta H_{298K} = -306KJ/mole$

Carbon

Assumptions:

- All reactions are considered as conversion reactions.
- Heat exchanger is used instead of boiler, since there is no provision of boiler in DWSIM.
- Heater is used in place of fired heater, since there is no provision of fired heater in DWSIM.

Process Description:

- The propylene feed (Stream 1) is heated in Propylene Heater and brought up to a temperature of 545℃.
- The chlorine (Stream 2) is mixed with the hot propylene in a Jet Mixer and then the mixed reactant stream (Stream 3) at 511℃ is fed to the Reactor.
- The reaction is isothermic in nature, thus Stream 4 is at 511℃.
- The gases leaving the reactor (Stream 4) contain unreacted propylene along with the reaction products like allyl chloride, chloropropene and di-chloropropene.
- These hot gases (Stream 4) are cooled in a waste-heat boiler (Boiler) using Boiler Feed Water at 90℃ and the outlet stream (MSTR-019) at 200℃ leaves the waste-heat boiler.
- Then, the outlet stream (MSTR-019) enters the heat exchanger (Heat Exchanger), where it is cooled using cooling water (Cooling Water In), and the outlet stream (Stream 5) is sent for further processing, including the refining of the allyl chloride and the separation and recycle of unused propylene.

Process Flowsheet:

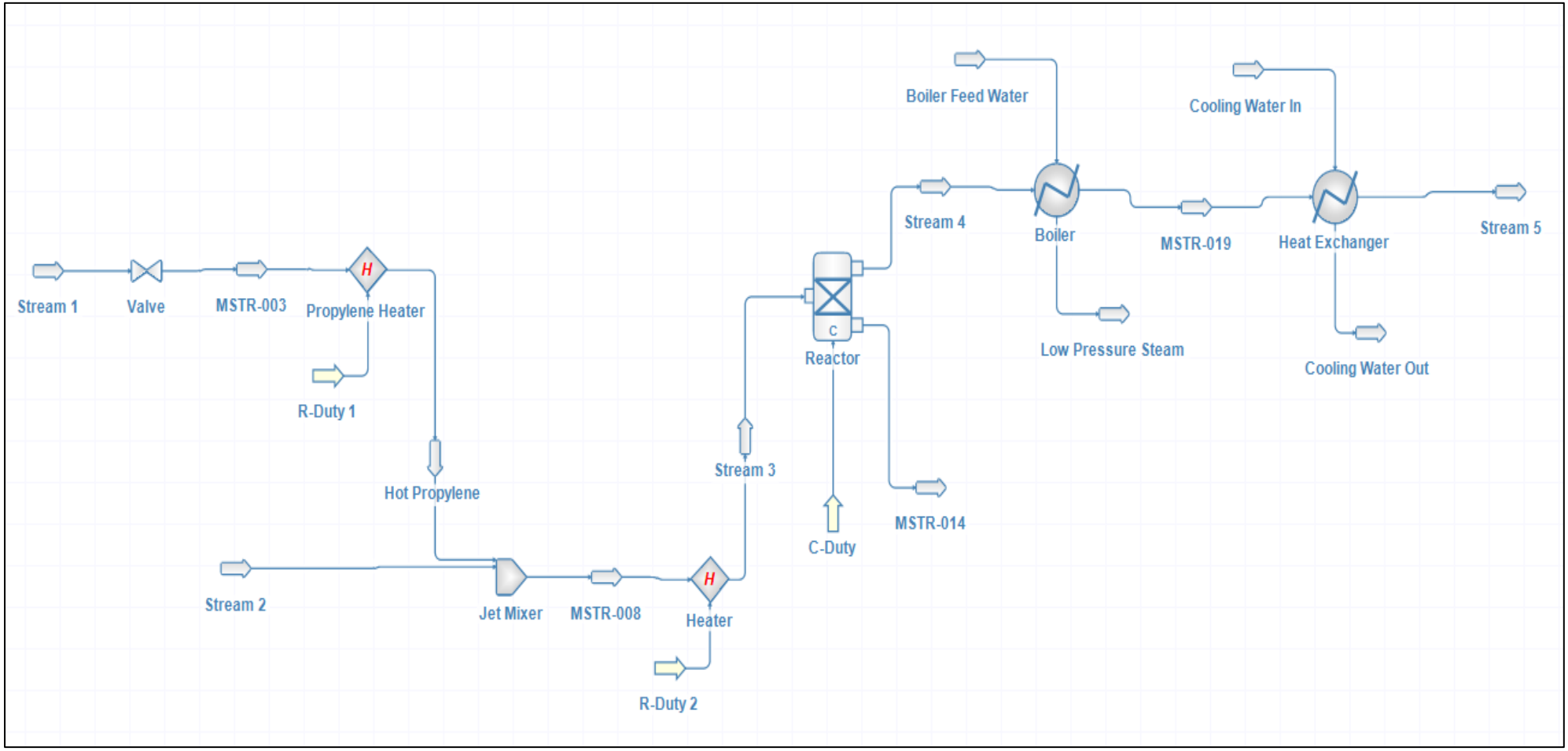

Figure 1: Production of Allyl Chloride

Summary:

Components	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5
Temperature (K)	298.44737	298.15	784.15	784.15	323.15
Pressure (Pa)	1170000	644000	304000	277000	209000
Mass Flow rate (kg/s)	0.88706347	0.38800792	1.2750714	1.2750714	1.2750714
Molar Flow rate (mol/s)	21.080556	5.4722222	26.552778	27.208036	27.208036
Mixture Molar Fraction					
Propylene	1	0	0.7939115	0.58799728	0.58799728
Chlorine	0	1	0.2060885	0	0
Allyl Chloride	0	0	0	0.15880261	0.15880261
2-Chloro prop-1-ene	0	0	0	0.018478406	0.018478406
3,3-Dichloro prop-1-ene	0	0	0	0.0046976834	0.0046976834
Hydrogen chloride	0	0	0	0.21557471	0.21557471
Water	0	0	0	0	0
Carbon	0	0	0	0.014449314	0.014449314

Reference:

1. Wen, C. Y., and Y. H. Yu, "A Generalized Method for Predicting Minimum Fluidization Velocity," AIChE J. 12, no. 610 (1966).