Production of Chlorobenzene from Chlorine And Benzene

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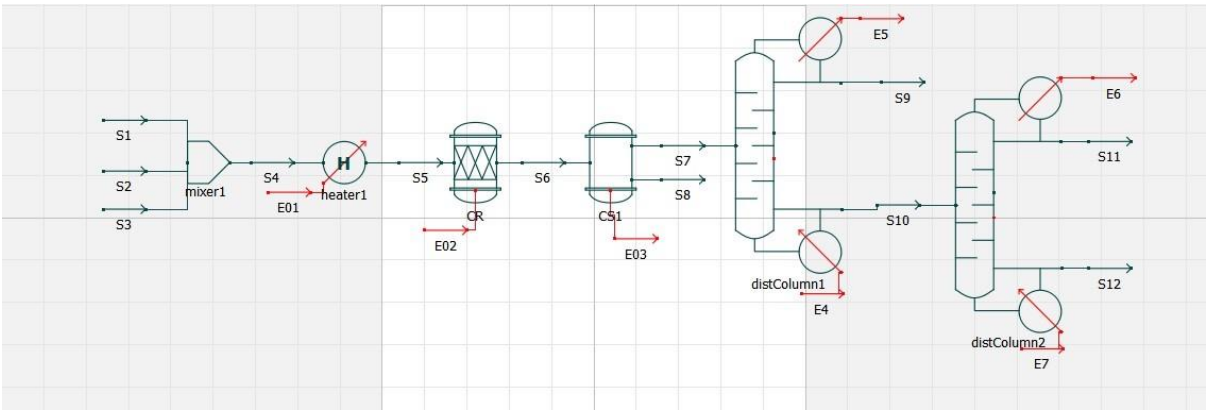
Background

Chlorinated Aromatic Hydrocarbons plays a significant role by acting as a precursor in various production process. One such important chlorinated aromatic hydrocarbon is monochlorobenzene which is predominately used in the production of intermediates such as nitrophenol, nitrophenetole and used in other applications such as paints, adhesives, dyes, and drugs as it is a high boiling solvent.

Monochlorobenzene is industrially prepared by reaction of chlorine and liquid benzene with the help of Lewis acids like $FeCl_3, AlCl_3, MnCl_2$ which acts as a catalyst. During the production hydrogen chloride is obtained as the byproduct and other undesirable compound such as Ortho and Para Dichlorobenzene is produced. The amount of production of dichlorobenzene depends on the ratio of benzene and chlorine chosen. Hence to achieve desired amount of monochlorobenzene complete conversion of benzene is not intended. It is reported that we can obtain a maximum of 73 % of monochlorobenzene and 22-23 % of dichlorobenzene and 4-5 % of unreacted benzene under suitable conditions when chlorine and benzene is reacted. NRTL is most suitable thermodynamic package to simulate the production of monochlorobenzene.

Description of Flowsheet



Liquid benzene(S1), gaseous chlorine (S2) and the recycle stream (S3) is fed together as a feed. The feed is mixed with the help of mixer (mixer 1) and then heated to around 313.15 K using a heater (heater1). The stream is then fed into the conversion reactor where chlorine and benzene react to form monochlorobenzene, hydrogen chloride, o-dichlorobenzene, and p-dichlorobenzene. The product mixture is then introduced into the compound separator where the components like hydrogen chloride and chlorine is separated into material stream (S8) completely. The stream (S7) which is rich in monochlorobenzene is sent to a distillation column (DistColumn1) to separate the unreacted benzene (S9) that is present. The unreacted benzene can be recycled and used for further processing. The stream (S10) is rich in monochlorobenzene is subjected to another distillation

column (Distcolumn2) to separate from the dichlorobenzene and obtain around 94-95% purity in the stream (S11) which is the required product.

Results

Stream	S1	S2	S3	S6	S8	s11
Temperature(K)	313.15	313.15	357.921	313.15	313.15	406.38
Pressure (Pa)	101325	101325	101325	101325	101325	101325
Mole Flows(mol/s)	12.8022	14.1032	2.2364	29.1418	14.103	10.4546
Molar Composition						
Benzene	1	0	0.82265	0.080503	0	0.00022
Chlorine	0	1	0	0.000425	0.0008797	4.44E-16
Hydrogen Chloride	0	0	2.59E-19	0.483525	0.9912	0
Monochlorobenzene	0	0	0.17683	0.374825	0	0.956088
o-dichlorobenzene	0	0	0.00037	0.022537	2.465E-32	0.01113
p-dichlorobenzene	0	0	0.176832	0.03863	0	0.032579

Comments and Conclusion

A flowsheet is built to produce chlorobenzene using chlorine and benzene. A product of high purity is obtained using this process. The same flowsheet was simulated in DWSIM which resulted in less than 1% error.

Reference

(1) Uwe Beck and Eckhard Loser, Chlorinated Benzenes and other Nucleus-Chlorinated Aromatic Hydrocarbons in Ullmann's Encyclopedia of Industrial Chemistry, Vol. 8 (2010), pp. 488- 491.

(2) Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Emissions from Chlorobenzene Production, Chapter 4 in LOCATING AND ESTIMATING AIR EMISSIONS FROM SOURCES OF CHLOROBENZENES (REVISED), March 1994.