Process Development for the Production of 6 TPD of Styrene from Benzene and Ethylene

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A. Background

Styrene is the raw material for the manufacture of a number of commodity and functional thermoplastic and thermosetting resins such as polystyrene, Styrene-butadiene, Acrylonitrile butadiene styrene and so on. Styrene is also known as Ethyl benzene, Vinyl benzene, and Phenyl ethene. Styrene is a colorless oily liquid and gives a sweet smell on evaporation. Approximately 25 million tons of styrene was produced in 2010[1].

B. Description of Flow Sheet

The feed containing equi-molar composition of Benzene and Ethylene was preheated to reaction temperature of 95°C [2] at constant pressure of 1.01325 bar. Then the feed was fed to a conversion reactor which produces Ethyl Benzene at 70% conversion with respect to Benzene. The product stream from the conversion reactor containing Ethyl Benzene and unreacted Ethylene and Benzene was sent to a distillation column. In the distillation column Ethyl Benzene was obtained as bottom product and the distillate stream contains small amount of Ethyl Benzene and unreacted Ethylene and Benzene. The purified Ethyl Benzene, obtained as bottom product was then heated to 650°C[2] and was fed to an equilibrium reactor which produces Styrene, Hydrogen and unreacted Ethyl Benzene. The exit stream from the equilibrium reactor was cooled to 40°C and then fed to a gas-liquid separator where Hydrogen was removed as vapour stream. The liquid stream containing Ethyl Benzene and Styrene was heated to 50°C and then sent to another distillation column where 99.94 % pure Styrene was obtained as the bottom product and Hydrogen and unreacted Ethyl Benzene as the top products. The stream obtained as top product was split into two separate streams and recycled, owing to convergence error of the recycle block, in order to increase the productivity of the process. Finally the product obtained was cooled to room temperature.

C. Results

The process flow sheet for the production of 6 TPD of Styrene at a temperature of 650°C and at 1 bar pressure was simulated. Since the kinetics of both the reactions was not known a conversion of 70% was assumed in the "conversion reactor" in DWSIM. Two shortcut distillation columns were simulated to calculate the actual number of stages, minimum number of stages, location of feed stage and minimum reflux ratio for the given light key and heavy key compositions. In the first shortcut distillation column, Benzene is taken as the light key component and Ethyl Benzene is taken as the heavy key component. The light key composition at the bottoms is fixed at 0.01, the heavy key composition in the distillate is fixed at 0.01 and a reflux ratio of 5 was assumed for the first shortcut column. The shortcut column was simulated and a minimum reflux ratio of 0.17 was obtained with actual number of stages equal to 5. In the second shortcut distillation column, Ethyl Benzene is taken as the light key component and Styrene is taken as the heavy key component. The light key composition at the bottoms is fixed at 0.01, the heavy key composition in the distillate is fixed at 0.001 and a reflux ratio of 7 was assumed. The shortcut column was simulated and a minimum reflux ratio of 2.16 was obtained with actual number of stages equal to 38. The results from both the shortcut distillation columns were used to specify the parameters required for the simulation of rigorous distillation column. The first rigorous distillation column was operated at a condenser pressure of 20.5 bar and reboiler pressure of 0.3 bar. Product flow rate of 2.79 kmol/h and a reflux ratio of 5 were assumed. Similarly, the second rigorous distillation column was operated at a condenser pressure of 5 bar and reboiler pressure of 0.95 bar. Product flow rate of 2.4102 kmol/h and a reflux ratio of 13 were assumed. A desired product flow rate of 251 kg/h was obtained which corresponds to 6 TPD of Styrene.

Results			
Object	S-1	S-19	
Temperature	25	25	C
Pressure	1.01325	0.95	bar
Mass Flow	500	251.02286	kg/h
Molar Flow	9.419034	2.4102	kmol/h
Molar Fraction (Mixture) / Benzene	0.5	2.6646209E-24	
Molar Fraction (Mixture) / Ethylene	0.5	6.3623822E-78	
Molar Fraction (Mixture) / Ethylbenzene	0	0.00060502009	
Molar Fraction (Mixture) / Hydrogen	0	1.8267088E-104	
Molar Fraction (Mixture) / Styrene	0	0.99939498	

D. Conclusion and Recommendation

This study shows that open source process simulator can be used for simulating process and development of process flow sheets. This work can be extended to simulate production of Polystyrene by including the polymerization reaction. Further, a conversion reactor can be replaced with a kinetic reactor from rate law kinetics obtained from experiments.

Unit System: (Custom 5 in DWSIM)

Temperature - °C

Pressure - bar

Molar Flow Rate – kmol/h

Mass Flow Rate – kg/h

Volumetric Flow Rate – m^3/h

Density – kg/m^3

References

1. https://en.wikipedia.org/wiki/Styrene
2. http://nptel.ac.in/courses/103103029/24