Production of Toluene from n-heptane

Madhur Wadhwani
Department of Chemical Engineering
Ujjain Engineering College, Ujjain
E-mail: madhurwadhwani14@gmail.com

Background & Description:

Toluene, also known as methylbenzene, is an organic chemical compound. It is a colourless, water-insoluble liquid. Toluene is a very good solvent because, unlike water, it can dissolve many organic compounds. In many commercial products, toluene is used as a solvent that in paint thinners, nail polish remover, glues, and correction fluid.

Beyond this toluene has many other uses in different industries too. In the explosives industry, it is essential in making the flammable, explosive compound known as TNT or trinitrotoluene. In the plastics industry, it is a component in the manufacturing of nylon and plastic bottles. Hair dyes and nail products include toluene, as well, utilized by the cosmetics industry.

Statement:

Toluene is produced from n-heptane by dehydrogenation over a Cr_2O_3 catalyst:

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_3 \rightarrow C_6H_5CH_3 + 4H_2$$

The toluene production process is started by heating n-heptane from 65 to 800 ºF in a heater. It is fed to a catalytic reactor, which operates isothermally and converts 15 mol% of the n-heptane to toluene. Its effluent is cooled to 65 ºF and fed to a separator (flash). Assuming that all of the units operated at atmospheric pressure.

Assumptions:

1. Feed is pure n-heptane.
2. Process is operating at atmospheric pressure.
3. There is no pressure drop in reactor and heat exchanger.
4. A conversion of 15% is set.
5. Custom units is used in simulation and not in SI unit system.

Process description:

According to statement, a feed of pure n-heptane (100 lbmole/hr) at temperature of 65 ºF, is fed to heater, where it is heated to 800 ºF. Now this heated stream(R-Feed) is fed to reactor

where conversion occurs and 15% n-heptane is converted to toluene and hydrogen according to reaction stoichiometry. The reactor is operating at a temperature of 800 ºF. This product is stream is passed through a cooler from where it is cooled to 65 ºF and then finally fed (Separator-Feed) to flash separator, where it separates out to vapour (major hydrogen content) and liquid stream.

As in flowsheet a large amount of energy is utilized in heating from 65 ºF to 800 ºF and cooling the same from 800 ºF to 65 ºF. From calculated results, nearly same amount of energy is exchanged. Thus, a specification block is employed to utilize the energy of high temperature reactor outlet in heating the feed. Thus reducing the energy content required.

Results:

Material stream							
Object	Feed	Liquid	R-Feed	R-Product	Separator-	Vapour	
Temperature	65	65	800	800	65	65	F
Pressure	14.696	14.696	14.696	14.696	14.696	14.696	psi
Mass Flow	10020.2	9628.09	10020.2	10020.2	10020.2	392.109	lbm/h
Molar Flow	100	97.3676	100	160	160	62.6324	lbmol/h
Volumetric Flow	0.064931	0.060338	25.4086	40.8017	6.72429	6.66395	ft3/s
Mixture Specific Enthalpy	-160.618	-162.494	426.368	436.036	-156.76	-15.9554	BTU/lbm

Energy stream			
Object	E-01	E-03	
Energy Flow	5.94E+06	5.94E+06	BTU/h

References:

Problem statement- **Simulation of Process Equipment by using Hysys by Trupti Ambar, Tyagee Chavan, Manali Kavale, S M Walke**

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Theory- Wikipedia/toluene

Study.com/toluene