Hydroalkylation of Toluene to Benzene Using Hydrogen

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ABSTRACT

Hydroalkylation is a chemical reaction that often involves reacting an aromatic hydrocarbon, such as toluene in the presence of hydrogen gas to form a simple aromatic hydrocarbon devoid of functional groups. This chemical process usually occurs at high temperature, at high pressure, or in the presence of a catalyst.

Hydroalkylation of toluene is synergized by poly-isopropyl benzene which is obtained in the process of manufacture of cumene as distillate. The process is to obtain benzene from dealkylation in the presence of H2. In the process, the pure benzene of 96.43% is obtained while about 96.7% of Toluene is recycled back to the feed stream. Various hydroalkylation processes can be used, in which hydrogen and alkyl aromatic hydrocarbons are contacted in a reaction zone at high temperature.

Key words: Hydroalkylation-Toluene-Benzene-DWISM-Simulation

PROCESS DESCRIPTION

The property package used for the complete flow Diagram is SRK Model.

Hydrogen and Toluene are fed in their respective feed streams and are mixed in the mixer (MIX-012) and the mixture feed is obtained from the material stream (MSTR-010). The mixture product passes through the heater (HEAT-004) where calculations are based on outlet of 873.15K and efficiency is 100%.

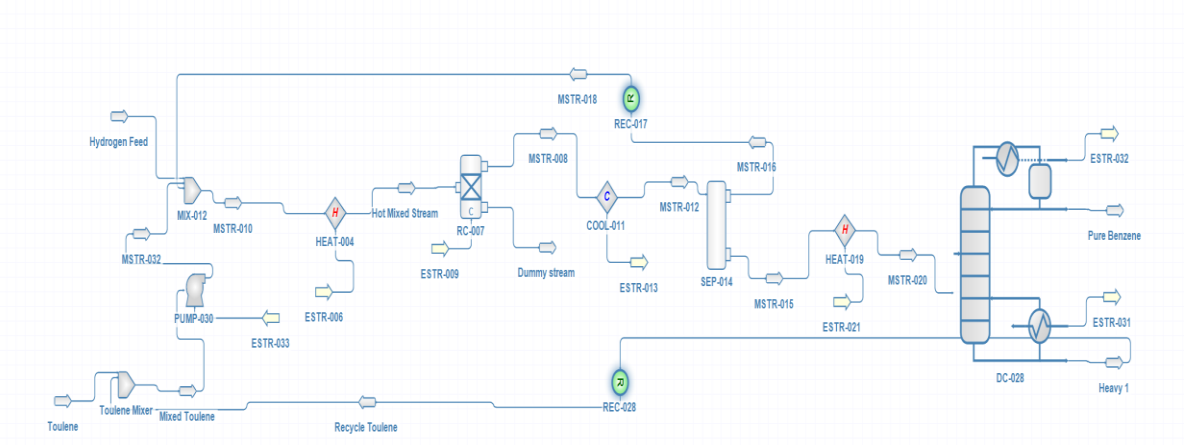
The hot mixture from heater is fed to the conversion reactor RC-007. In the reactor, Toluene is reacted with hydrogen to produce Benzene and Methane.

Toluene + Hydrogen→Benzene + Methane

Reactor operates at 600-650˚C and 35-40 atms, product stream from the reactor is passed through a cooler (COOL-011) of outlet temperature of 353.15K with efficiency of 100%. The products are then separated in the separator vessel where vapour stream and light liquid streams are separated to MSTR-016 and MSTR-015 respectively. The vapour is recycled back to the mixture while the light liquid stream is passed through the heater HEAT-019, with the outlet temperature of 375.15. The product is then fed to the distillation column (DC-028).

From the distillation column, Pure Benzene is obtained as a distillate while Toluene is recycled back to Toluene mixture. The Toluene recycled and Toluene fed are pumped to the mixture MIX012.

The Flowsheet and Results Table



Results Table

Object	Toluene	Recycled Toluene	Pure Benzene	MSTR-020	MSTR-016	MSTR-008	Hot Mixed Stream	Heavy 1	
Temperature	373.15	541.97	474.65	373.15	353.15	873.15	873.15	541.97	K
Pressure	2E+5	2.35E+06	2.35E+06	2.35E+06	2.35E+06	2.35E+06	2.35E+06	2.35E+06	Pa
Molar Flow	30.55	0.53	28.14	28.68	6.61E3	6.64E3	6.64E3	0.534	mol/s
Molar Fraction of Components									
Hydrogen	0	3.08E-14	6.27E-3	6.16E-3	0.453	0.451	0.456	3.08E-14	
Toluene	1	0.967	1.26E-3	1.926E-2	4.285E-4	5.09E-4	5.098E-3	0.967	
Benzene	0	0.032	0.964	0.947	0.0520	0.0558	0.0512	0.0325	
Methane	0	7.019E-13	0.0280	0.0275	0.494	0.492	0.487	7.019E-13	
Biphenyl	0	0	0	0	0	0	0	0	

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