HYDRO DEALKYLATION for TOLUENE

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INTRODUCTION

The hydrodealkylation of toluene1 (HDA) is a process used to produce BENZENE , METHANE and DIPHENYL . Hydrodealkylation is a chemical reaction that often involves reacting an aromatic hydrocarbon, such as toluene, in the presence of hydrogen gas to form a simpler aromatic hydrocarbon devoid of functional groups. Another example is the conversion of 1,2,4-trimethylbenzene to xylene.

DESCRIPTION OF THE FLOWSHEET

The main reaction in the process is:

$$Toluene + H_2 ----------> Benzene + CH_4$$
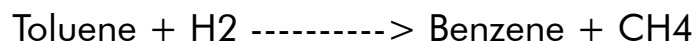
Toluene and hydrogen are converted in aconversion reactor to produce benzene and methane. Typically the reaction reaches a conversion of 70%. The reaction is highly exothermic and the typical operating conditions are 600 C to 660 C, and 35-40 bar.

The HDA process begins with mixing fresh toluene , recycle unreacted toluene,hydrogen and the recycle product from the flash separator. The mixing is achieved in a storage tank. Product stream from mixer is sent to a heat exchanger to heat the stream.The mixture is preheated before it is introduced to the heater or furnace. In the furnace the stream is heated to 625.516 C, the reaction temperature, then introduced into the reactor. The reactor is where the main reaction happens:

$$C_7H_8 + H_2 ------------> C_6H_6 + CH_4$$
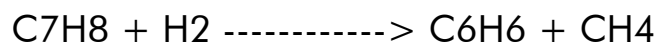
This reaction is irreversible. Another minor side reaction2 is often observed:

$$2 Benzene --------------> Diphenyl + H_2$$
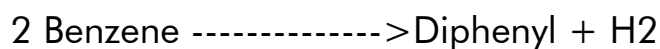
The product stream from the reactor is sent to the same heat exchanger and then quenched to get temperature 150-170 C and then sent to a separator which operates at 32.8 bar and 38 C .The botttom from the separator is sent to the distallation column 1 to separate METHANE as a top product ,this diastillation column is Demath-

aniser.The bottoms from the demathaniser is sent to the distillation column 2 to separate is BENZENE as a top product .The bottoms from the latter is sent to a distillation column 3 to separate BIPHENYL as a bottom product and the recycle stream of Toluene is pumped to the mixer.The product from the separator is perged and one stream is compressed and sent to mixer as a recycle stream.

Results obtained from the flowsheet

RESULTS								
Object	TOP	TOLUENE REC	TOLUENE	METHANE	HYDROGEN	BIPHENYL	BENZENE	
Temperature	34.2731	110.732	26.8019	-213.044	38	240.492	80.1783	C
Pressure	32.8	1.01325	38.3	10	38.3	1.01325	1.01325	bar
Mass Flow	21645.1	4216.56	15387.5	165.676	909.978	499.788	12282	kg/h
Molar Flow	2111.02	45.4555	166.999	10.6296	333	3.26728	157.216	kmol/h
Molar Fraction (Mixture) / Toluene	0.000866523	0.990004	1	1.56637E-07	0	0.0195516	0.00052794	
Molar Fraction (Mixture) / Biphenyl	2.14926E-07	0.01	0	4.10209E-36	0	0.980257	3.54926E-54	
Molar Fraction (Mixture) / Benzene	0.00824487	3.14397E-06	0	0.029	0	1.42891E-08	0.999472	
Molar Fraction (Mixture) / Hydrogen	0.453934	1.50549E-161	0	0.160912	0.9489	2.44027E-172	1.53063E-52	
Molar Fraction (Mixture) / Methane	0.536955	2.45481E-161	0	0.810111	0.0511002	1.71232E-172	1.30991E-50	

References

Flowsheet   : https://www.cocosimulator.org/index_sample.html
OR https://www.cocosimulator.org/downloads/HDA_preview.gif

Thoery : https://www.cpp.edu/~tknguyen/che304/Homework/Hydrodealkylation%20Simulation.doc