

## Production of Benzene via the hydrodealkylation of Toluene

Main reaction: Toluene + Hydrogen  $\rightarrow$  Benzene +Methane

Reaction Conditions : 600 -650 deg C, 20 to 60 bar

Catalysis: Chromia on porous carrier

The process flow diagram for the process is shown in Figure 1.

The fresh toluene feed (no.1) along with recycle stream (no.11) is pressurized and mixed with hydrogen (no.3 and no. 5). The mixture is fed to a heater (E-101) followed by furnace heater (H-101) to increase the temperature to around 600 deg C. The heated stream (no.4) along with a small fraction of recycled hydrogen stream (no. 7) is introduced into a packed bed catalytic reactor (R-101). The reactor effluents are cooled and fed to phase separators (V-102 and V-103) to separate unreacted hydrogen along with product methane. A part of the separated gases is recycled back and the rest is collected as fuel gas (no.16). The liquid stream (no. 10) from the second phase separator is fed to distillation column after passing through the feed heater (E-103). The distillation column separates the light key component (benzene) which is subsequently cooled and stored (no.15). The bottom heavy component (toluene) is recycled back to the toluene vessel.

The following points need to be noted while creating this flowsheet in DWSIM:

- a) A single heat exchanger was used to raise the feed temperature to the reaction temperature as there are no provisions of fired heater in DWSIM
- b) The side reactions were ignored
- c) The reactor operation was considered isothermal
- d) One pass conversion of 75% was used for simulation
- e) The three recycle loops (Two for hydrogen and one for toluene) were used. However, they were found to be extremely sensitive to the guess values fed to the solver and solutions were not converging. The initial guess values were improved by trial and error.
- f) The data given in Turton et al, 2013 was used as the basis to create the sheet and confirm the simulation results from DWSIM
- g) Instead of V-104, a phase separator was used to allow separation of vapors (no.19)

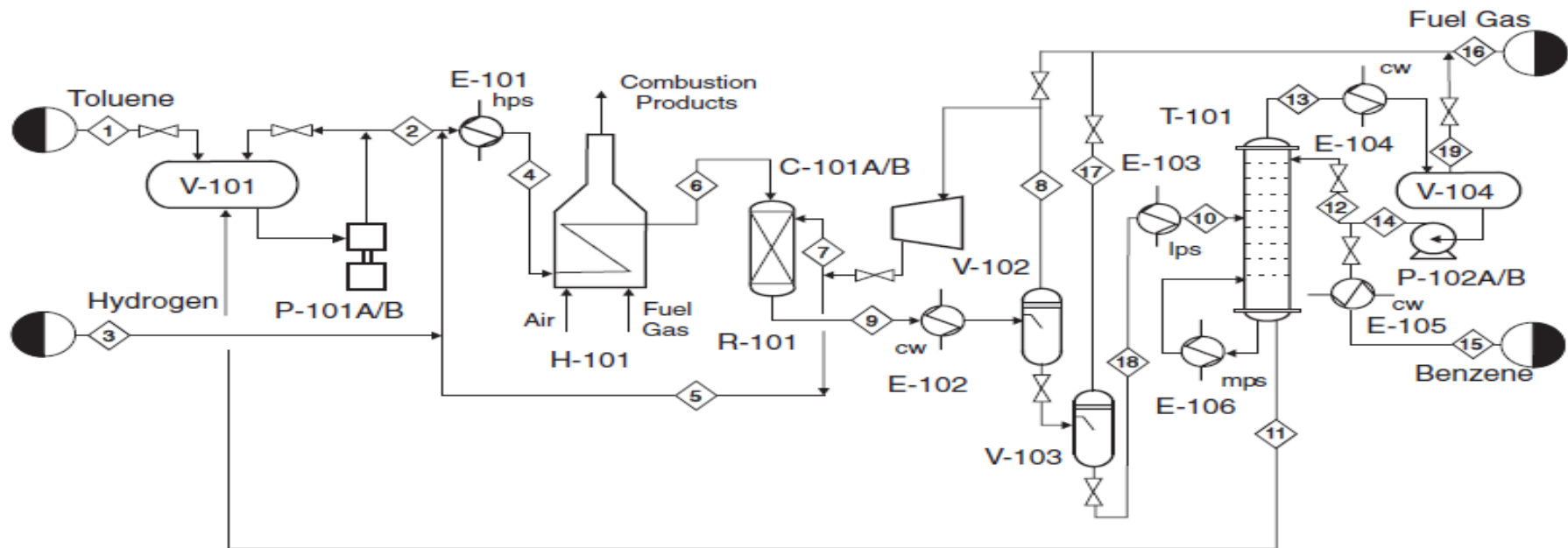


Figure 1: Production of benzene via hydrodealkylation of toluene

## RESULTS

Parameter	Units	INPUT		OUTPUT	
		toluene	Hydrogen	cooled benzene	fuel gas
Temperature	C	24.8	24.8	38	38.2
Pressure	bar	2	25.5	2.5	2.5
Mass Flow	kg/h	9,972	820	8,229	2,563
Molar Flow	kmol/h	108.3	301.7	105	305
<b>Mole fractions</b>					
Toluene		0.996	0	0.0001	0.000782
Hydrogen		0.000	0.95	0	0.588154
Methane		0.000	0.05	0	0.402231
Benzene		0.004	0	0.99	0.008833