Production of Styrene.

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A. Background

Styrene is hydrocarbon. It is formed by gaseous reaction. Petrochemical industries manufacture Styrene. Styrene is used for SBR rubber and resins. By two ways, Styrene can be manufactured: (a) Dehydrogenation of Ethylbenzene (b) Hydrogenation-dehydrogenation of Acetophenone. The first route is considered for this project.

B. Description of flow-sheet

Fresh Ethyl Benzene and Steam is mixed using mixer. Then it passes through Heat Exchanger. Here, stream temperature reaches 487 ^{0}C. This stream mixes with steam and passes through reactor. From reactor, products and byproducts are formed. Then it passes thorough heater and 2nd reactor. Another reactor's product heat is integrated with 1st reactor's feed. Reactor feed is then cooled with cooler and decanted into decanter. Here, lighters, heavier and gas stream are separated. Organic phase is then sent to distillation column. In 1st distillation column, pure styrene gets from the bottom and lighters got from the top. In 2nd distillation column, Ethyl Benzene gets from the bottom and Benzene + Toluene mixture got from the top.

C. Result

Reactor-1: Ethyl Benzene conversion: 45 %
Water conversion: 2%

Reactor-2: Ethyl Benzene conversion: 45 %
Water conversion: 2.5%

Distillation column-1 (Product-Bottom): 12498.12 kg/hr (Total)
12491.61 kg/hr (Styrene)

Distillation column-2 (Bottom): 7404.88 kg/hr (Total)
6026.04 kg/hr (Ethyl Benzene)
1378.8 kg/hr (Styrene)

Distillation column-2 (Top): 2941.92 kg/hr (Total)
987.12 kg/hr (Benzene)
732.96 kg/hr (Styrene)

D. Conclusion

Styrene production process can be simulated in DWSIM and given product purity can be achieved.

E. Recommendation

i. Use below figures for reference.

ii. Last 2 reactions can't be considered because CO amount is <1 %.

iii. 2nd distillation column bottom can't be recycled because it is off-specification.

iv. Strictly DWSIM 5.5 used because previous version has error: given key was not present in dictionary. Error solved due to mailed to Daniel Wagnner.

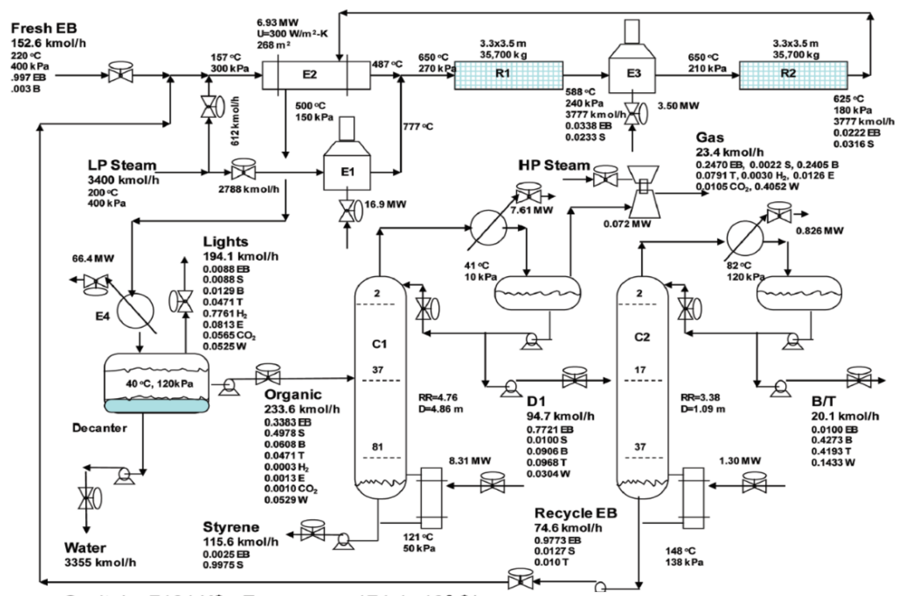
F. Units

Mass flow: kg/s

Molar flow: kmol/hr

Temperature: ^{0}C

Pressure: kPa



$$C_6H_5CH_2CH_3 \leftrightarrow C_6H_5CHCH_2 + H_2 \quad (1)$$

$$C_6H_5CH_2CH_3 \rightarrow C_6H_6 + C_2H_4 \quad (2)$$

$$C_6H_5CH_2CH_3 + H_2 \rightarrow C_6H_5CH_3 + CH_4 \quad (3)$$

$$2H_2O + C_2H_4 \rightarrow 2CO + 4H_2 \quad (4)$$

$$H_2O + CH_4 \rightarrow CO + 3H_2 \quad (5)$$

$$H_2O + CO \rightarrow CO_2 + H_2 \quad (6)$$

Figure Reference: IIT Bombay

$$\mathcal{R}_{1F} = p_{EB}k_{1F}e^{-E_{1F}/RT}$$
$$\mathcal{R}_{1R} = p_S p_W k_{1R}e^{-E_{1R}/RT} \quad (7)$$

Table 1. Reaction Kinetics[a]

	k	E (kJ/kmol)	concentration (Pascals)
reaction 1 forward	0.044	90 981	P_{EB}
reaction 1 reverse	6×10^{-8}	61 127	$P_S P_H$
reaction 2	27,100	207 989	P_{EB}
reaction 3	6.484×10^{-7}	91 515	$P_{EB} P_H$
reaction 4	4.487×10^{-7}	103 997	$(P_W)^2 P_E$
reaction 5	2.564×10^{-6}	6723	$P_W P_M$
reaction 6	1779	73 638	$P_W P_{CO}$

[a] Overall reaction rates have units of kmol s^{-1} m^{-3}.

$$\mathcal{R}_2 = p_{EB}k_2e^{-E_2/RT} \quad (8)$$

$$\mathcal{R}_3 = p_{EB}p_H k_3e^{-E_3/RT} \quad (9)$$

$$\mathcal{R}_4 = p_W(p_E)^{0.5}k_4e^{-E_4/RT} \quad (10)$$

$$\mathcal{R}_5 = p_W p_M k_5e^{-E_5/RT} \quad (11)$$

$$\mathcal{R}_6 = p_W p_{CO} k_6e^{-E_6/RT} \quad (12)$$