Styrene mass balance problem

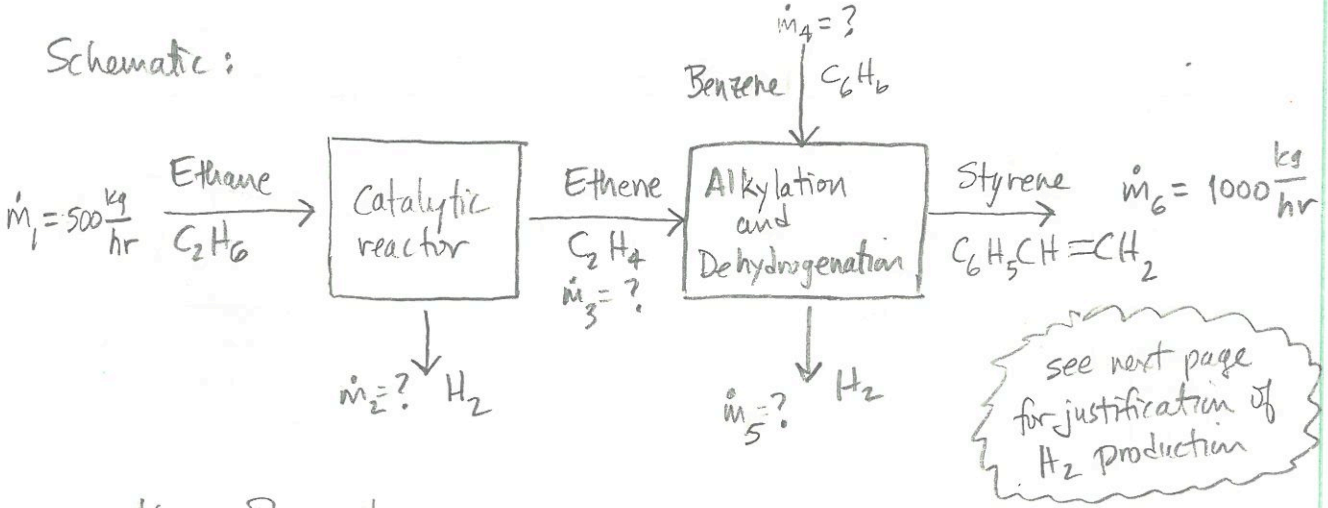
Step 1 GIVEN: Available supply of ethane: $\dot{m}_{C_2H_6} = 500 \ \mathrm{kg/hr}$

Desired production of styrene: $\dot{m}_{styrene} = 1000 \ \mathrm{kg/hr}$

FIND: Required supply of Benzene: $\dot{m}_{C_6H_6} = ?$

Rate of H_2 production: $\dot{m}_{H_2} = ?$

Step 2 Schematic:



see next page for justification of H_2 production

Known Parameters:

$\dot{m}_1 = 500 \frac{kg}{hr}$ = mass flow rate of Ethane (input)

$\dot{m}_6 = 1000 \frac{kg}{hr}$ = mass flow rate of Styrene (output)

$\mathcal{M}_H = 1 \frac{kg}{k\text{-mol}}$ = molar mass of H

$\mathcal{M}_C = 12 \frac{kg}{k\text{-mol}}$ = molar mass of C

$\Rightarrow \mathcal{M}_{C_2H_6} = 2 \times 12 + 6 \times 1 = 30 \frac{kg}{k\text{-mol}}$ = molar mass of Ethane

$\mathcal{M}_{C_2H_4} = 2 \times 12 + 4 \times 1 = 28 \frac{kg}{k\text{-mol}}$ = molar mass of Ethene

$\mathcal{M}_{C_6H_6} = 6 \times 12 + 6 \times 1 = 78 \frac{kg}{kmol}$ = molar mass of Benzene

$\mathcal{M}_{C_6H_5CH=CH_2} = 8 \times 12 + 8 \times 1 = 104 \frac{kg}{kmol}$ = molar mass of Styrene

SIDEBAR: How do you know that H_2 is produced by the two reactions in the schematic?

To answer that question, consider each reaction separately.

① Catalytic production of Ethene from Ethane

$$\underbrace{C_2H_6}_{2C+6H} \rightarrow \underbrace{C_2H_4}_{2C+4H}$$

} As written here, there is an imbalance in the number of Hydrogen atoms on the two sides of the reaction

To balance the reaction, H_2 must be produced

$$\underbrace{C_2H_6}_{2C+6H} \longrightarrow \underbrace{C_2H_4 + H_2}_{2C+6H}$$

② Alkylation of Ethene and Benzene to form Styrene

$$\underbrace{C_2H_4 + C_6H_6}_{8C+10H} \longrightarrow \underbrace{C_6H_5CH=CH_2}_{8C+8H}$$

NOT Stoichiometric

The left hand side (reactants) have 2 more H atoms than the right hand side

To balance the reaction, H_2 must be produced

$$\underbrace{C_2H_4 + C_6H_6}_{8C+10H} \longrightarrow \underbrace{C_6H_5CH=CH_2 + H_2}_{8C+10H}$$

Unknowns : $\dot{m}_2$ = H_2 production from the catalytic converter

$\dot{m}_5$ = H_2 production from the Alkylation and Dehydrogenation reaction

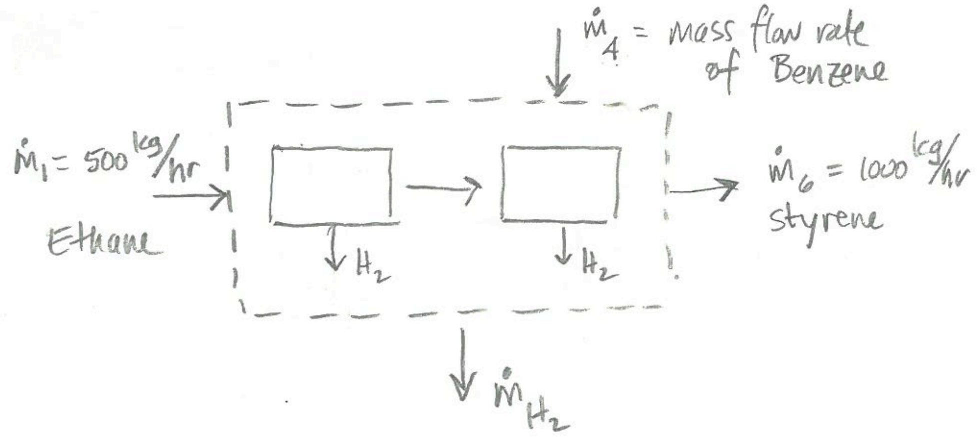
<u>Note</u>: Only $\dot{m}_2 + \dot{m}_3 = \dot{m}_{H_2}$ = total H_2 production is needed

more unknowns : $\dot{m}_3$ = flow rate of Ethene

$\dot{m}_4$ = required input flow rate of Benzene

<u>Key Observation</u>: We only need to find the total rate of H_2 production and the required input of Benzene. We are not interested in the intermediate product, Ethene.

Therefore, we can treat the two reactions as a single process. Redraw the system schematic.



This new schematic shows the two unknowns $\dot{m}_4$ and $\dot{m}_{H_2}$

<u>Step 4</u> This is a steady flow process

There is no generation or consumption of the material, i.e. the total mass of H and total mass of C are conserved.

$$\Rightarrow \dot{m}_{in} = \dot{m}_{out} \text{ overall and for C and H}$$

Step 5:

Overall Mass Balance

$$\dot{m}_{in} = \dot{m}_{out}$$

$$\dot{m}_{Ethane} + \dot{m}_{Benzene} = \dot{m}_{H_2} + \dot{m}_{Styrene}$$

or, using symbols

$$\dot{m}_1 + \dot{m}_4 = \dot{m}_{H_2} + \dot{m}_6 \qquad (1)$$

Carbon Mass Balance:

In any stream, the mass flow rate of Carbon is equal to the total mass flow rate <u>of that stream</u> times the fraction of carbon in the stream.

Therefore, at the Ethane input

$$\dot{m}_{C,Ethane} = \frac{24}{30}\dot{m}_1$$

$24 \frac{kg}{kmol}$ = contribution of C to molar mass of C_2H_6

$30 \frac{kg}{kmol}$ = molar mass of C_2H_6

∴ The mass flow rate of carbon in the Ethane input stream is $\frac{24}{30}\dot{m}_1$

Repeat the preceding analysis while performing a mass balance on the Carbon

$$\underset{\underset{\text{Ethane}}{\nearrow}}{\frac{24}{30}\dot{m}_1} + \underset{\underset{\text{Benzene}}{\uparrow}}{\frac{72}{78}\dot{m}_4} = \underset{\underset{\text{Hydrogen}}{\uparrow}}{0\,\dot{m}_{H_2}} + \underset{\underset{\text{Styrene}}{\nwarrow}}{\frac{96}{104}\dot{m}_6} \qquad (2)$$

Step 6

Equations (1) and (2) are two equations for the two unknowns $\dot{m}_4$ and $\dot{m}_{H_2}$

But, Equation (2) has only one unknown, $\dot{m}_4$ (since the multiplier of $\dot{m}_{H_2}$ is zero)

Solve Equation (2) for $\dot{m}_4$

$$\frac{72}{78}\dot{m}_4 = \frac{96}{104}\dot{m}_6 - \frac{24}{30}\dot{m}_1$$

$$\dot{m}_4 = \frac{78}{72}\left(\frac{96}{104}\dot{m}_6 - \frac{24}{30}\dot{m}_1\right)$$

$$= \frac{78}{72}\left[\underbrace{\frac{96}{104}\left(1000\,\frac{kg}{hr}\right) - \frac{24}{30}\left(500\,\frac{kg}{hr}\right)}_{523\ kg/hr}\right]$$

$$\therefore \boxed{\dot{m}_4 = 566.7\,\frac{kg}{hr}}$$ mass flow rate of Benzene

Substitute the value of $\dot{m}_4$ into Equation (1) to solve for $\dot{m}_{H_2}$

$$\dot{m}_{H_2} = \dot{m}_1 + \dot{m}_4 - \dot{m}_6$$

$$= 1000\,\frac{kg}{hr} - 566.7\,\frac{kg}{hr} - 500\,\frac{kg}{hr}$$

$$\therefore \boxed{\dot{m}_{H_2} = 66.7\,\frac{kg}{hr}}$$ mass flow rate of H_2

Step 7

CHECK: Use H_2 mass balance to check the computations

$$\underset{\underset{\text{Ethane}}{\uparrow}}{\frac{6}{30}}\dot{m}_1 + \underset{\underset{\text{Benzene}}{\uparrow}}{\frac{6}{78}}\dot{m}_4 = \dot{m}_{H_2} + \frac{8}{104}\underset{\underset{\text{Styrene}}{\nwarrow}}{\dot{m}_6}$$

$$\dot{m}_{in} = \dot{m}_{out} \Rightarrow \dot{m}_{in} - \dot{m}_{out} = 0$$

$$\frac{6}{30}\left(500\,\frac{kg}{hr}\right) + \frac{6}{78}\left(566.7\,\frac{kg}{hr}\right) - 66.7\,\frac{kg}{hr} - \frac{8}{104}\left(1000\,\frac{kg}{hr}\right) \overset{?}{=} 0$$

$$100\,\frac{kg}{hr} + 43.59\,\frac{kg}{hr} - 66.7\,\frac{kg}{hr} - 76.92\,\frac{kg}{hr} \overset{?}{=} 0$$

$$\underbrace{-0.03\,\frac{kg}{hr} \overset{?}{=} 0}_{\text{OK with roundoff errors in the calculations}}$$