<u>CHAPTER-4</u>

<u>MATERIAL BALANCE</u>

<u>Basis:</u> 1 hour (Oxo-Reactor)

100 K-moles of Propylene

R = (Synthesis reactor + Unreacted Propylene) per K-mole of Propylene feed.

x= mole fraction of Propylene in the Stripped gas.

Propylene feed = (100 + 100 Rx) =100(1+Rx) K- moles

Amount of Unreacted Propylene = 100(1+Rx) x 0.02 = 2(1+Rx) K -moles

Synthesis gas = 100 R (1 –x) K -moles

<u>Assume :</u> 100% of Unreacted Propylene is stripped in the striper.

Propylene : Synthesis gas = 1 : 2

$$\therefore \quad \frac{100(R)\,(1-x)}{100\,(1+Rx)} = 2 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

$$\frac{R\,(1-x)}{1+Rx} = 2$$

$$R-Rx = 2+2Rx$$

$$3Rx = R - 2$$

$$x = \frac{(R-2)}{3R}$$

$$x = \frac{2\,(1+Rx)}{2(1+Rx) + 100\,R(1-x)} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

$$x = \frac{(1+Rx)}{(1+Rx) + 50R(1-x)} = \frac{1+Rx}{1+Rx + 50R - 50Rx} = \frac{1+Rx}{1+50R - 49Rx}$$

$$x(1+50R - 49Rx) = 1 + Rx$$

$$x + 50Rx - 49Rx^2 = 1 + Rx$$

$$x + 49Rx - 49Rx^2 = 1$$

$$x\{1 + 49R - 49Rx\} = 1$$

$$\frac{(R-2)}{3R}\left\{1 + 49R - \frac{49R(R-2)}{3R}\right\} = 1$$

$$(R-2)(98R + 101) = 9R$$

$$98R^2 + 101R - 196R - 202 = 9R$$

$$98R^2 - 104R - 202 = 0$$

a = 98, b = -104, c = -202

$$R = \frac{+(104) \pm \sqrt{(-104)^2 - 4(98)(-202)}}{2(98)} = \frac{104 \pm \sqrt{90000}}{2(98)}$$

$\therefore$ R = 2.061

$$\therefore x = \frac{(R-2)}{3R} = \frac{(2.061 - 2.0)}{3(2.061)} = \frac{0.061}{6.183} = 0.0099$$

Synthesis gas = 100 R(1-x) = 100 x 2.061(1-0.0099) = 204.6 K-moles

Propylene = 100(1+Rx) = 100 {1+2.061(0.0099)} = 102.03 K- moles

Off- gas (Unreacted synthesis gas) = 204.06 – 102.03

= 102.03 K-moles

98% of Propylene is converted.

∴K-moles of Butyraldehyde = 0.98 x 102.03 = 99.99 K-moles

n-Butyraldehyde : iso-Butyraldehyde = 4 : 1

∴K-moles of n- butyraldehyde = 99.99 x 0.8 = 79.992 K – moles

6% n- butyraldehyde of is converted to n-butanol

∴K-moles of n-butanol = 0.06 x 79.992

= 4.800 K-moles

K-moles of iso- butyraldehyde = 99.99 – 79.992 = 19.998 K-moles

4% of iso- butyraldehyde is converted to iso-butanol

∴K-moles of iso-butanol = 0.04 x 19.998
= 0.800 K-moles

Distillation column (I) : Aldehydes/Alcohol separator

Assume: all Aldehydes (both n & iso- butyraldehydes leave as the top product) and all alcohols (both n and iso-butanol leave as bottom product).

Distillation column (II) :

Feed: n-Butyraldehyde = 79.992 – 4.800 = 75.192 K-moles
iso-butyraldehyde = 19.998 – 0.800 = 19.198 K-moles

More volatile component -------------------------- iso- butyraldehyde
(mass balance on the basis of more volatile component)

$$Z_F = \frac{19.198}{94.39} = 0.203\ ; \quad x_D = 0.987\ ; \quad x_W = 0.012$$

<u>Over balance</u>**:**

$F = D + W$

$D = F – W = 94.39 – W$

<u>Component balance:</u>

$F\ Z_F = Dx_D + W.x_{w.}$

94.39(0.203) = (94.39 – W) (0.987) + W(0.012)

19.161 = 93.163 – 0.987W + 0.012W

0.975W = 93.163 –19.161 = 74.002

$$W = \frac{74.002}{0.975} = 75.9 \quad \text{K-moles}$$

$\therefore$ D = 94.39 – 75.90 = 18.49 K-moles

n-Butyraldehyde in W	=	0.988 x 75.9	=	74.989 K-moles
iso-Butyraldehyde in W	=	75.9 - 74.989	=	0.911 K- moles

<u>Aldol condensation</u>: (90% conversion efficiency)

$$\text{K-moles of 2-Ethyl hexanol} = \frac{0.90 \times 74.989}{2} = 33.745 \text{ K-moles}$$

Side stream = water + Unreacted n-Butyraldehyde + iso-butyraldehyde

= 33.745 + 0.1 (74.989) + 0.911

= 33.745 + 7.499 + 0.911

= 42.155 K- moles

Hydrogenation : (99% conversion)

K-moles of 2-Ethyl hexanol = 0.99 x 33.745 = 33.408 K-moles

H_2 required (considering 100% excess) = 2 x (2 x 33.745) =134.98 K-moles

Propylene	2-ethyl hexanol
102.83	33.408

Production required :50,000 tons/year

Molecular weight of 2-Ethyl hexanol = 130.23

Operating period (per anum) = 8000 hours

$$\therefore \text{Production (K-moles/hr)} = \frac{50000 \times 1000}{8000 \times 130.23} = 47.99 \text{ K-moles}$$

$$\therefore \text{K-moles of Propylene required} = \frac{47.99 \times 102.03}{33.048} = 146.564 \text{ K-moles}$$

∴Synthesis gas required = 2 x 146.564 = 293.13 K-moles

Unreacted propylene = 0.02 x 146.564 = 2.931 K- moles

Off gas = 293.13 – 146.564 = 146.564 K-moles

K-moles of butyraldehyde = 0.98 x 146.564 = 143.633 K-moles

K-moles of n-butyraldehyde = 143.633 x 0.8 = 114.91 K-moles

K -moles of n-butanol formed = 0.06 x 114.91 = 6.89 K-moles

K-moles of iso-butyraldehyde = 143.633 – 114.91 = 28.723 K-moles

K-moles of iso-butanol = 0.04 x 28.723 = 1.149 K-moles

Distillation column:

Feed: n- butyraldehyde = 114.91 - 6.89 = 108.02 K-moles

iso-butyraldehyde = 28.723 - 1.149 = 27.574 K- moles

F = 108.02 + 27.574 = 135.594 K-moles

$$Z_F = \frac{27.574}{135.594} = 0.203$$

Overall Balance:

F=D+W

D = F – W = 135.594 – W

Component balance:

$FZ_F = Dx_D + Wx_w$

135.594 (0.203) =(135.594 - W) (0.987) + W (0.012)

27.526 =133.831 – 0.975 W

W = 109.03 K- moles

n- butyraldehyde in W = 0.988 x 109.03 = 107.72 K- moles

iso- butyraldehyde in W = 109.03 – 107.72 = 1.31 K- moles

K- moles of 2-Ethylhexanal = $\frac{0.90 \times 107.72}{2}$ = 48.474 K- moles

Side stream = 48.474 + 0.1 (107.72) + 1.31

= 60.556 K- Moles

K- moles of 2-ethyl hexanol = 0.99 x 48.474

= 47.99 K- moles

H_2 = 2 x (2 x 48.474) = 193.869 K-moles.