MATERIAL BALANCE

The beginning of any design problem is to quantify the different streams involved in the process. This is done by formulating a material balance for the different units of the plant. The basis for the material balance is the product of **100 tons per day (TPD) of ISOAMYL ALCOHOL** at a purity of 99mol%. The mass/molar flow rates of different streams and their composition are given below.

Data Available:

Molecular weight of Isoamyl Alcohol= **88.15** kg/kmol.

Molecular weight of Valeraldehyde =**86.08** kg/kmol.

Molecular weight of Isobutylene = **56.00** kg/kmol.

Molecular weight of Carbon monoxide= **28.00** kg/kmol.

Molecular weight of Hydrogen = **2.00** kg/kmol.

Now,

100 TPD of Isoamyl alcohol = $\frac{100\times1000}{24\times88.15}$

= 47.2679 kmol/hr.

= 4166.6667 kg/hr.

Thus, 100 TPD Isoamyl alcohol = 47.2679 kmol/hr.

BASIS: 1 HOUR OPERATION.

From the stoichiometry of reactions, it is clear that 1mole of Isoamyl alcohol is produced by using 1 mole of Isobutylene.

Therefore, to produce 47.4679 kmol of Isoamyl alcohol amount of Isobutylene required is 47.2679 kmol or 2647.0024 kg. , provided the yield is 100%.

Thus, for a yield of 80%,

Amount of Isobutylene required = $\frac{47.3679}{0.80}$

= 59.0849 kmol/hr.

= 3303.7544 kg/hr.

Therefore, amount of Isobutylene actually required = 59.0849 kmol/hr.

=3308.7544 kg/hr.

Let the ratio of hydrogen to carbon monoxide be **1.2:1.0**

i.e., **H_2: CO:: 1.2:1.0**

Amount of CO required = 59.0849 kmol/hr.

= 1654.3772 kg/hr.

Amount of Hydrogen required =1.2×59.0849

=70.9019 kmol/hr.

=141.8038 kg/hr.

Assuming catalyst concentration be 1wt%.

To calculate the amount of catalyst required:

Let the amount of catalyst present be "X" kg.

Thus, we have

$$\frac{X}{[(59.0849\times56) + (59.0849\times28) + (70.9019\times2) + X]} = 0.01$$

i.e.,

$$\frac{X}{[5104.9354 + X]} = 0.01$$

i.e., $X= 0.01(5104.9354+X)$

i.e., $X= (0.01\times5104.9354) + (0.01\times X)$

i.e., $(1-0.01) \times X= 0.01\times5104.9354$

i.e.,

$$X = \frac{(0.01\times5104.9354)}{0.99}$$

i.e., X= 51.5650 kg.

Therefore amount of catalyst required = 51.5650 kg.

4.1 MATERIAL BALANCE AROUND THE REACTOR:

REACTION:

$$\underset{\text{Isobutylene}}{(CH_3)_2\text{-}C= CH_2} + \underset{\text{Synthesis Gas}}{(CO+ H_2)} \longrightarrow \underset{\text{Valeraldehyde}}{(CH_3)_2\text{-}CH\text{-}CH_2\text{-}CHO}$$

Conversion=95%, Temperature= 170^0C to 175^0C

Selectivity =80%. Pressure= 250 atmospheres.

Raw materials:

Synthesis Gas: CO = 59.0849 kmol/hr.

H_2 =70.9019 kmol/hr.

Isobutylene = 59.0849 kmol/hr.

Cobalt catalyst = 51.5650 kg.

Now,

Amount of Valeraldehyde produced= 59.0849×0.95×0.80

= 44.9045 kmol/hr.

=3865.3794 kg/hr.

Amount of Isoamyl alcohol formed= 59.0849×0.95×0.20

=11.2262 kmol/hr.

= 989.5834 kg/hr.

Amount of Carbon monoxide used = 44.9045+ 11.2261 …… (From stoichiometry)

= 56.1306 kmol/hr.

= 1571.6568 kg/hr.

Amount of Carbon monoxide left unused= 59.0849- 56.1306

=2.9543 kmol/hr.

= 82.7204 kg/hr.

Also from stoichiometry we have,

Amount of Isobutylene used = 56.1306 kmol/hr.

= 3143.3136 kg/hr.

Thus, amount of Isobutylene left unused =59.0849-56.1306

= 2.9543 kmol/hr.

= 165.4408 kg/hr.

{Amount of Hydrogen used for

the production of Valeraldehyde} = 70.9019×0.95×0.80

= 53.8854 kmol/hr.

= 107.7709 kg/hr.

{Amount of Hydrogen used for

the production of Isoamyl alcohol} = 70.9019×0.95×0.20

= 13.4714 kmol/hr.

= 26.9427 kg/hr.

Total amount of Hydrogen used = 53.8854 + 13.4714

= 67.3568 kmol/hr.

= 134.7136 kg/hr.

Amount of Hydrogen remaining unused = 70.9019-67.3568

= 3.5451 kmol/hr.

= 7.0902 kg/hr.

Output from the Oxo Reactor:

Alcohol = 11.2261 kmol/hr. = 989.5807 kg/hr.

Valeraldehyde= 44.9045 kmol/hr. = 3865.3794 kg/hr

Isobutylene = 2.9543 kmol/hr. = 165.4408 kg/hr.

Carbon Monoxide= 2.9543 kmol/hr. = 82.7204 kg/hr.

Hydrogen = 3.5451 kmol/hr. = 7.0902 kg/hr.

Cobalt catalyst = 51.561 kg.

Assuming that in the catalyst separator, complete separation of catalyst, vent gases (CO and H_2) and Isobutylene and (alcohol + valeraldehyde) takes place. Further, it is assumed that the catalyst is completely recycled back to the Oxo Reactor.

Further, it is assumed that (CO + H_2) and Isobutylene are 5% in the separator.

4.2 MATERIAL BALANCE AROUND THE CATALYST SEPERATOR:

Input to the catalyst separator:

Alcohol = 11.2261 kmol/hr.

Valeraldehyde= 44.9045 kmol/hr.

Isobutylene = 2.9543 kmol/hr.

Carbon Monoxide= 2.9543 kmol/hr.

Hydrogen = 3.5451 kmol/hr.

Cobalt catalyst = 51.561 kg.

Output from the Catalyst Separator:

Amount of Catalyst recycled back to Oxo reactor = 51.561 kg.

Vent Gases: Carbon Monoxide = (1-0.05) ×2.9543

= 2.8066 kmol/hr.

= 78.5848 kg/hr.

Hydrogen = (1-0.05) ×3.5451

= 3.3679 kmol/hr.

= 6.7358 kg/hr.

Isobutylene = (1-0.05) ×2.9543

= 2.8066 kmol/hr.

= 157.1696 kg/hr.

Amount of Alcohol from Separator to the Hydrogenation Reactor = 11.2261 kmol/hr.

= 989.5807 kg/hr.

{Amount of Valeraldehyde from the Separator

to the Hydrogenation Reactor} = 44.9045 kmol/hr.

= 3865.3794 kg/hr.

4.3 MATERIAL BALANCE AROUND THE HYDROGENATION REACTOR:

REACTION:

$(CH_3)_2$-CH-CH_2-CHO + H_2 --------------> $(CH_3)_2$-CH-CH_2-CH_2-OH

Valeraldehyde Isoamyl Alcohol

Conversions = 85% Temperature= 150^0C

Selectivity =100% Pressure= 100 atmospheres.

Input to the Hydrogenation Reactor from the separator:

Alcohol = 11.2261 kmol/hr.

Valeraldehyde= 44.9045 kmol/hr.

Now, from the stoichiometry, we have,

{Amount of Alcohol produced from

44.9045 kmoles of Valeraldehyde} = 44.9045 ×0.85 ×1.0

= 38.1688 kmol/hr.

= 3364.5797 kg/hr.

Thus,

Total amount of Alcohol produced= 38.1688 + 11.2261

= 49.3949 kmol/hr.

= 4354.1604 kg/hr.

Amount of Valeraldehyde remained unused = 44.9045 × (1-0.85)

= 6.7357 kmol/hr.

= 579.8091 kg/hr.

Let the amount of hydrogen entering the Hydrogenation Reactor be 1.50 times the stoichiometry.

Therefore, amount of Hydrogen entering = 1.50 ×44.9045

= 67.3568 kmol/hr.

= 134.7136 kg/hr.

Amount of Hydrogen used in the production of alcohol = 44.9045 ×0.85 ×1.0

= 38.1688 kmol/hr.

= 76.3376 kg/hr.

Thus, amount of Hydrogen left unused = 67.3568 - 38.1688

= 29.1880 kmol/hr.

= 58.3760 kg/hr.

Output from the Hydrogenation Reactor:

Isoamyl Alcohol = 49.3949 kmol/hr.

Valeraldehyde = 6.7357 kmol/hr.

Hydrogen= 29.1880 kmol/hr.

Assuming that all the hydrogen remaining unreacted in the Hydrogenation Reactor is separated from the alcohol plus aldehyde mixture completely and is recycled back to Hydrogenation Reactor from the Separator.

4.4 MATERIAL BALANCE AROUND THE SEPARATOR:

Input to the Separator from the Hydrogenation Reactor:

Isoamyl Alcohol = 49.3949 kmol/hr.

Valeraldehyde = 6.7357 kmol/hr.

Hydrogen = 29.1880 kmol/hr.

Output from the separator:

{Hydrogen recycled back to

the Hydrogenation Reactor} = 29.1880 kmol/hr.

= 58.3760 kg/hr.

Isoamyl Alcohol = 49.3949 kmol/hr.

= 4354.1604 kg/hr.

Valeraldehyde = 6.7357 kmol/hr.

= 579.8091 kg/hr.

The mixture of Valeraldehyde and Isoamyl alcohol from the Separator is fed to a Distillation Column.

4.5 MATERIAL BALANCE AROUND THE DISTILLATION COLUMN:

Input to Distillation Column from the Separator:

Isoamyl Alcohol = 49.3949 kmol/hr.

Valeraldehyde = 6.7357 kmol/hr.

Let "F" represents the Feed, which is a mixture of Isoamyl alcohol and Valeraldehyde.

"D" represents the Overhead product/Distillate, which is Valeraldehyde.

"W" represents the Bottom product/ Residue, which is Isoamyl alcohol.

"X_F" represents the mole fraction of Valeraldehyde in Feed.

"Y_D" represents the mole fraction of Valeraldehyde in Distillate/ Overhead Product.

"X_W" represents the mole fraction of Valeraldehyde in Residue/ Bottom Product.

Overall material balance:

$$F = D + W \qquad \text{-------} \ (1)$$

Now,

Feed=F= 49.3949 + 6.7357 =<u>56.1306</u> kmol/hr.

Thus,

$$X_F = \frac{6.7357}{56.1306} = \underline{0.12}$$

Let $X_W = \underline{0.01}$

Therefore,

$$W = \frac{47.2679}{0.99} = \underline{47.7454} \text{ kmol/hr.}$$

Therefore, D= F-W = 56.1306- 47.7454 = <u>8.3852</u> kmol/hr.

Component Balance:

$$(F \times X_F) = (D \times Y_D) + (W \times X_W) \qquad \text{------} \ (2)$$

Therefore,

$$Y_D = \frac{(F \times X_F) - (W \times X_W)}{D} \qquad \text{----------} \ (3)$$

i.e., $$Y_D = \frac{(56.1306 \times 0.12) - (47.7454 \times 0.01)}{8.3852}$$

i.e., $Y_D = \underline{0.7465.}$

Thus, we have

F = <u>56.1306</u> kmol/hr. $X_F = \underline{0.12}$

D = <u>8.3852</u> kmol/hr. $Y_D = \underline{0.7465}$

W= 47.7454 kmol/hr. X_W = 0.01

The subsequent sections concerning the Energy Balance and Design of Equipment are based on the above material balance. The material balance is an ideal balance, neglecting the losses