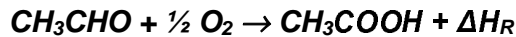


HEAT BALANCE FOR ACETIC ACID PLANT:



The above reaction is carried out at liquid phase.

From Perry 7th edition,

$$\Delta H_{F,g} \text{ acetaldehyde at } 25^\circ\text{C} = -166.2 \text{ KJ/mol}$$

$$\Delta H_{F,g} \text{ acetic acid at } 25^\circ\text{C} = -432.8 \text{ KJ/mol}$$

$$\lambda_{\text{acetaldehyde at } 25^\circ\text{C}} = 24.474 \text{ kJ/mol}$$

$$\lambda_{\text{acetic acid at } 25^\circ\text{C}} = 23.2989$$

Now, ΔH_R of the above reaction in liquid phase at 25°C can be given as follows.

$$\begin{aligned} \Delta H_{R,25^\circ\text{C}} &= \text{PRODUCT} - \text{REACTANT} \\ &= [(-432.8 - 23.2989) - (166.2 - 24.474)] \\ &= -265.425 \text{ kJ/mol} \end{aligned}$$

As the reaction temperature maintained is at 75°C , where the liquid phase estimated heat capacities at different temperature are:

$$C_P \text{ of acetaldehyde at } 75^\circ\text{C} = 123909.825 \text{ J/kmol}^\circ\text{k}$$

$$C_P \text{ of AA at } 75^\circ\text{C} = 129761.21 \text{ J/kmol}^\circ\text{k}$$

$$C_P \text{ of oxygen at } 50^\circ\text{C} = 29476.915 \text{ J/kmol}^\circ\text{k}$$

$$\begin{aligned} \Delta H_{R,75^\circ\text{C}} &= \Delta H_{R,25^\circ\text{C}} + \Sigma(\gamma_i * C_{Pi})|_{\text{PRODUCT}} - \Sigma(\gamma_i * C_{Pi})|_{\text{REACTANT}} \\ &= -266.425 * 10 + (123910 - (129761.2 + 0.5 * 29477)) \\ &= -266.454 \text{ kJ/mol} \end{aligned}$$

REACTOR HEAT BALANCE:

$$\Delta H_{R,75^{\circ}\text{C}} = -266.454 \text{ kJ/mol}$$

Now, 10% dilution = $10 \times 32/28 = 11.43\%$ by vol. of O_2
by wt. of O_2

Now, as conversion (x) = 0.938

Feed rate of acetaldehyde = 173.61 kmol/hr

Feed rate of O_2 (10% dil.) = 165.08 kmol/hr

Also, the flue stream to the scrubber contains 15.9%
acetaldehyde by weight.

∴ Unconverted O_2 leaving

$$\begin{aligned} \text{the reactor} &= (165.08 \times 0.8857) - (173.61 \times 0.5 \times 0.938) \\ &= 64.79 \text{ kmol/hr} \end{aligned}$$

and unreacted N_2

$$\text{leaving} = 18.87 \text{ kmol/hr}$$

∴ Total flue gas leaving reactor = 83.66 kmol/hr

∴ Avg.mol.Wt.of } = $4.79 \times 32/3.66 + 18.87 \times 28/83.66$

the flue gas } = 31.082 kg/kmol

∴ flue gas containing 15.9%

acetaldehyde by wt. = 0.118

Now, λ of acetaldehyde

at 5atm pressure and $75^{\circ}\text{C} = 19.66 \text{ kJ/kmol}$

ρ of acetaldehyde at $75^{\circ}\text{C} = 15.951 \text{ kmol/m}^3$

ρ of acetic acid at $75^{\circ}\text{C} = 16.472 \text{ kmol/m}^3$

ρ of water at $75^{\circ}\text{C} = 54.137 \text{ kmol/m}^3$

Stream out	Wt. fraction (%)	Mole fraction, x (%)
Acetic acid	94.0	86.02
Water	3.6	10.98
Acetaldehyde	2.4	3.0

Also, as the reactor volume is constant,

Volumetric flow rate in = Volumetric flow rate out

$$\text{Volume of feed in} = 173.61/15.951 = 10.883 \text{ m}^3/\text{hr}$$

Assuming, ideal solution, the average volume of the outgoing-stream

$$\begin{aligned} &= (0.8602/16.472 + 0.1098/54.137 + 0.03/15.951)^{-1} \\ &= 17.763 \text{ kmol/m}^3 \end{aligned}$$

$$\begin{aligned} \therefore \text{Avg. mol. Wt.} &= 0.8602 \cdot 60 + 0.1098 \cdot 18 + 0.03 \cdot 44 \\ &= 54.9084 \text{ kg/kmol} \end{aligned}$$

Now, feed from reactor to the first

$$\begin{aligned} \text{distillation column} &= 5633.73 \cdot 6250/3600 = 9780.78 \text{ kg} \\ &= 178.129 \text{ kmol} \end{aligned}$$

$$\therefore \text{Volume output} = 178.129/17.763 = 10.028 \text{ m}^3$$

$$\begin{aligned} \therefore \text{Acetaldehyde lost with flue gas} &= 129.16 \text{ kmol/day} \\ &= 5.382 \text{ kmol/hr} \end{aligned}$$

But, the actual evaporation should

$$\text{be more than that} = 20 \cdot 5.382 \text{ kmol/hr} = 107.64 \text{ kmol/hr}$$

\therefore In the reactor,

$$\begin{aligned} \text{Heat generated during reaction} &= (173.61 \cdot 10^3 \cdot 0.938 \cdot 266.454) \\ &= 43.391 \cdot 10^6 \text{ kJ/hr} \end{aligned}$$

Again, heat required to evaporate

$$\begin{aligned} \text{acetaldehyde} &= (107.64 \cdot 10^3) \cdot 19.66 \\ &= 2.1162 \cdot 10^6 \text{ kJ/hr} \end{aligned}$$

HEAT BALANCE AROUND CONDENSER

Assume, the condenser being operated at the same pressure at that of the reactor = 5 atm.

$$\begin{aligned} \text{Here, the mole fraction of acetaldehyde in the stream leaving out with flue gas} \\ &= 107.64 / (107.64 + 18.87 + 64.79) \end{aligned}$$

$$= 0.5626$$

$$\begin{aligned}\therefore \text{Partial pressure acting on the acetaldehyde} &= 5 \times 0.5626 \\ &= 2.813 \text{ atm}\end{aligned}$$

Therefore, at this temperature, acetaldehyde will condensate at a temperature of **T = 54°C**, whereas the temperature of the reactor = **75°C**. Therefore, the reflux is sub-cooled.

Now, heat required to saturate

$$\text{the acetaldehyde to } 75^\circ\text{C} = 2.7579 \times 10^3 \text{ kJ/kmol}$$

$$\therefore \text{The total heat} = 19 \times 5.382 \times 2.7579 \times 10^3 = 0.282 \times 10^6 \text{ kJ/hr}$$

\therefore heat load to the condenser,

$$\lambda \text{ at } 54^\circ\text{C} = 21761.4 \text{ kJ/hr} = 618.13 \text{ kW}$$

Let, the acetaldehyde feed given at = 25°C

So, heat required to raise

$$\text{the acetaldehyde temperature to } 75^\circ\text{C} = 26.975 \times 10^3 \text{ kJ/hr}$$

\therefore The load on the reactor cooler

$$\begin{aligned}\text{i.e. } Q_{co} &= -2.1162 \times 10^6 - 0.282 \times 10^6 - 26.975 \times 10^6 + 43.391 \times 10^6 \\ &= 14.0178 \times 10^6 \text{ kJ/hr} = 3894 \text{ kW}\end{aligned}$$

Therefore, the flow out of the reactor contains

Acetic acid = 153.23 kmol/hr

Water = 19.56 kmol/hr

Acetaldehyde = 5.34 kmol/hr

In the *surge vessel*, the pressure drops from 5 atm to 1 atm. Assuming, it is an adiabatic process,

$$T_2 = T_1 \cdot (P_2/P_1)^{(R/C_p)}$$

where, C_p of the mixture at 75°C is calculated :

$$C_p = 0.8602 \cdot 136.813 + 0.03 \cdot 136.989 + 0.1098 \cdot 75.507 \\ 130.02 \text{ J/mol}^\circ\text{k}$$

$$\therefore T_2 = 314^\circ\text{k} = 41^\circ\text{C}$$

In calculating further properties, let us assume acetaldehyde presence is negligible.

$$\therefore \text{Acetic acid} = 0.8868$$

$$\therefore \text{Water} = 0.1132$$

Now, the top product from Ist distillation column contains acetic acid and water.

The temperature been calculated = 100.5°C

And the Ist distillation column been acting on a stripping column. Hence, there is no reflux. So, the product out is in vapor phase which is condensed and fed to the next column as saturated liquid.

$$\lambda_{AA} \text{ at } 101^\circ\text{C} = 23.899 \text{ kJ/mol}$$

$$\lambda_{\text{water}} \text{ at } 101^\circ\text{C} = 40.759 \text{ kJ/mol}$$

—

$$\lambda_{\text{Avg}} = (0.8868 \cdot 23.889 + 0.1132 \cdot 40.759) \text{ kJ/mol} \\ = 25.81 \text{ kJ/mol}$$

$$\therefore \text{Load on the condenser} = \left(\frac{4506.98}{(0.9234 \cdot 60 + 0.0766 \cdot 18)} \right) \cdot 6250 \text{ kmol} \\ 3600$$

$$\therefore Q = 137.79 \cdot 10^3 \cdot 25.81 \text{ kJ/hr} = 987 \text{ kW}$$

For the IInd distillation column:

—

$$h_f = F \cdot C_{pm} \cdot (T - T_R)$$

Let $T_R = 273.15^\circ\text{k}$ and $F = 141.63 \text{ kmol/hr}$

—

$$C_{pm} = (145.34 \cdot 0.9234 + 76.04 \cdot 0.0766) \text{ kJ/kmol}^\circ\text{k} \\ = 140.031 \text{ kJ/kmol}^\circ\text{k}$$

Again,

compositions	Acetic acid,X	Water,X
D ₁	0.293	0.707
D ₂	0.986	0.014
W	0.993	0.007

$$\begin{aligned} \therefore D_1 &= (174.52 / (0.293 \cdot 60 + 0.707 \cdot 18)) \cdot 6250 / 3600 \\ &= 9.998 \text{ kmol/hr at } T = 102.4^\circ\text{C} \end{aligned}$$

$$\therefore D_2 = 105.2 \text{ kmol/hr at } T = 118^\circ\text{C}$$

$$\therefore W = 21.3 \text{ kmol/hr at } T = 118^\circ\text{C}$$

$$\lambda D_1 = 35.82 \text{ kJ/mol}$$

$$\lambda D_2 = 24.135 \text{ kJ/mol}$$

$$R = 12.6$$

$$\begin{aligned} \therefore Q_c' &= (R + 1) \cdot 35.82 \cdot 9.998 \cdot 10^3 / 3600 \text{ kW} \\ &= 1352.93 \text{ kW} \end{aligned}$$

$$\begin{aligned} \therefore Q_c'' &= 24.135 \cdot 105.2 \cdot 10^3 / 3600 \text{ kW} \\ &= 705.38 \text{ kW} \end{aligned}$$