

5. ENERGY BALANCE

Basis : Per hour of operation

The gases viz. Propylene, propane, benzene enter at 25°C and benzene enters at 80°C.

To calculate the temperature of the mixture of gases after compression to 25 atm :

Cp values (J/mole K) at avg temperature of 53°C

Propylene 64.18

Propane 73.89

Benzene 82.22

Propylene in feed = 1105.09 kmoles/hr.

Benzene in feed = Benzene fed + recycled Benzene

$$= 1381.36 + 204.73$$

$$= 1586.09 \text{ kmoles/hr.}$$

Assuming that propylene is accompanied with propane as impurity in the ratio of 3:1.

Therefore propane in feed = 368.36 kmoles/hr.

Hence, $X_A = 0.3612$, $X_B = 0.5184$, $X_C = 0.1204$

$$C_p \text{ avg} = X_A C_{pA} + X_B C_{pB} + X_C C_{pC}$$

$$C_p \text{ avg} = 0.3612 \times 64.18 + 0.5184 \times 82.22 + 0.1204 \times 73.89$$

$$= 71.38 \text{ J/mole K}$$

Temperature of the stream after mixing :

Cp value J/kmole k at 30⁰ C

Propylene 64.52

Propane 70.17

Benzene 98.20

$$(1105.09 \times 64.52 + 1381.36 \times 98.20 + 368.36 \times 70.17) \times 10^3 \times (T-25)$$

$$= 204.73 \times 86.22 \times 10^3 \times (80-T)$$

or, $80 - T = 13.18 (T-25)$

or, $14.18 T = 409.5$

or, $T = 29^0 \text{ C}$

$$P_1=1 \text{ atm, } T_1= 29^0 \text{ C}$$

$$P_2= 25 \text{ atm, } \text{ To find } T_2$$

Considering isentropic process, we have

$$T_2 = T_1 (P_2 / P_1)^{(R / C_{p \text{ avg}})}$$

$$= 29(25 / 1)^{(8.314 / 71.38)}$$

$$= 42.19 \text{ } ^\circ\text{C}$$

$C_p \text{ avg at } 42.19 \text{ } ^\circ\text{C} \approx C_p \text{ avg at } 53 \text{ } ^\circ\text{C} = 71.38 \text{ J/ mole K}$

Assuming that the exit stream from pre-heater leaves at $100 \text{ } ^\circ\text{C}$

For the products from the reactor,

$$m = \text{cumene} + \text{DIPB} + \text{Benzene} + \text{propane}$$

$$= 1071.94 + 16.575 + 292.85 + 368.36$$

$$= 1749.72 \text{ kmoles/hr}$$

To find $C_p \text{ avg at } (250+100) / 2 = 175^\circ\text{C}$, $C_p \text{ J /mole K}$

Propane	107.76
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Cumene	205.24
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Di-isopropyl Benzene	302.97
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Propylene 97.60

Benzene 121.19

$$\begin{aligned}C_p \text{ avg} &= 0.6126 \times 205.24 + 0.0095 \times 302.97 + 0.1673 \times 121.19 \\ &\quad + 0.2105 \times 107.76 \\ &= 168.22 \text{ J/mole K}\end{aligned}$$

For the reactants leaving the pre-heater :

$m = \text{propylene} + \text{benzene} + \text{propane}$

$$= 1105.09 + 1586.09 + 368.36$$

$$= 3059.54 \text{ k moles/hr}$$

Heat balance around the pre-heater:

$$11749.72 \times 168.22 (250 - 100) \times 10^3 = 3059.54 \times 91.38 \times (T - 42.19) \times 10^3$$

$$T \approx 200 \text{ }^\circ\text{C}$$

The reactants have to be further heated to the reaction temperature of 250 °C before being fed to the reactor.

To find saturated steam required:

C_p avg of reactants has to be determined at $(200 + 250)/2 = 225 \text{ }^\circ\text{C}$

C_p value at average temperature of 225°C, J/kmole K

Propane 117.76

Propylene 97.60

Benzene 141.19

$$\begin{aligned}C_p \text{ avg} &= 0.3612 \times 97.60 + 0.5184 \times 141.19 + 0.1204 \times 117.76 \\ &= 122.62 \text{ J/mole K}\end{aligned}$$

$$m \text{ Cp avg}(250-100)=m_{\text{steam}} \lambda$$

$$3059.4 \times 122.62 \times 10^3 \times 150 = m_{\text{steam}} \times 2676$$

$$m_{\text{steam}} = 21.028 \times 10^6 \text{ kg /hr}$$

Energy balance around the reactor :

Enthalpy of reactants + heat evolved = Q + Enthalpy of products

$\Sigma m \text{ Cp dT reactants} + \text{heat evolved} = Q + \Sigma m \text{ Cp dT products}$

Heat evolved = 23.7683 K cal / g mole

$$= 99.3964 \text{ KJ/g mole}$$

Moles of cumene produced = 1072 k moles /hr

Heat evolved = 99.3964 x 1072 x 10³

$$= 106.63 \times 10^6 \text{ KJ/hr}$$

$\Sigma m \text{ Cp dT reactants} = 1105.09 \times 87.37 \times 10^3 (250 - 25) + 1586.09 \times 93.97 \times 10^3 (250 - 25) + 368.36 \times 97.34 \times 10^3 \times (250 - 25)$

$$= 6.3326 \times 10^{10} \text{ KJ/hr}$$

$\Sigma m \text{ Cp dT products} = 368.36 \times 10^3 \times (250 - 25) + 292.85 \times 93.97 \times 10^3 (250 - 25) + 1071.94 \times 10^3 \times 177.07(250 - 25) + 16.575 \times 10^3 \times 267.19 \times (250 - 25)$

$$= 5.796 \times 10^{10} \text{ KJ/hr}$$

$$\therefore 6.3326 \times 10^{10} + 106.63 \times 10^6 = Q + 5.796 \times 10^{10}$$

$$Q = 54.698 \times 10^8 \text{ KJ/hr}$$

To find propane requirement for quench :

Latent heat of vaporisation of propane liquid at 25 atm

(B.P = 68.4°C) = 0.25104 KJ/gm = 251.04 KJ/kg

Heat removal by propane heat quench :

Assuming that propane is removed completely in the depropanasing column and is sent for quenching .

Propane i.e recycled = 368.36 kmoles/hr

$$= 368.36 \times 44 \text{ kg/hr}$$

$$= 16207.84 \text{ kg/hr}$$

Cp of propane at T avg = $(250 + 68.4) / 2 = 159.2 \text{ }^\circ\text{C}$ is 2.56 KJ/kg $^\circ\text{C}$

$$Q = m \lambda + m C_p (250 - 68.4)$$

$$= 16207.84 \times (251.04 + 2.56 \times 181.6)$$

$$= 11.603 \times 10^6 \text{ KJ/hr}$$

$$\text{Additional heat to be removed} = 54.698 \times 10^8 - 11.603 \times 10^6$$

$$= 54.58 \times 10^8 \text{ KJ/hr}$$

$$= Q^1$$

Water is used for additional heat removal.

To find flow rate of water :

B.P. of water at 25 atm = 223.85 $^\circ\text{C}$

Latent heat of vaporisation = 2437 KJ/kg

Assuming that water at 25 $^\circ\text{C}$ is used for quenching

Cp of water at T avg = $(25+223.8)/2=124.43^\circ\text{C}$ is 3.7656 KJ/kg $^\circ\text{C}$

$$Q^1 = m C_p (223.85 - 25) + m \lambda$$

$$54.58 \times 10^8 = m (3.7656 \times 198.85 + 2437)$$

$$m = 1.713233 \times 10^6 \text{ kg/hr}$$

Distillation Column –1 :

To find the temperature at which the product stream is fed to distillation column –
1 :

$$\text{At } P_1 = 25 \text{ atm, } T_1 = 200 \text{ }^\circ\text{C}$$

$$\text{At } P_2 = 1 \text{ atm } T_2 = ?$$

$$\begin{aligned} C_p \text{ avg at } 100 \text{ }^\circ\text{C} &= 0.6126 \times 163.42 + 0.0095 \times 243.76 + 0.1673 \times 107.01 \\ &+ 0.2105 \times 79.47 \\ &= 137.05 \text{ J/gm mole} \end{aligned}$$

$$\begin{aligned} T_2 &= T_1 (P_2 / P_1)^{R/C_p \text{ avg}} \\ &= 100(1/25)^{8.314 / 137.05} \\ &= 82.26^\circ\text{C} \end{aligned}$$

This is further cooled to 25 °C and fed to the distillation column.

$$F=1749.72 \text{ kmoles/hr}$$

$$D=368 \text{ kmoles/hr}$$

$$W=1381.72 \text{ kmoles/hr}$$

Enthalpy of vapor that goes as overhead :

$$H_v = \text{Latent heat of vaporisation} + \text{sensible heat}$$

As propane is the major constituent that goes with the overhead, taking λ and C_p values of Propane,

$$H_v = V [\lambda + C_p (T_b - T_o)]$$

Assuming a reflux ratio of 0.5, we have $R=L/D = 0.5$

$$L=0.5 D = 0.5 \times 368 \times 44 = 8096 \text{ kg/hr}$$

$$V=L+D=8096+16192 = 24288 \text{ kg/hr}$$

Taking reference temperature as the temperature at which feed enters,

$$T_0 = 25 \text{ }^\circ\text{C} ; \quad T_b = 42.1 \text{ }^\circ\text{C} , \quad C_p = 2.41 \text{ KJ/kg }^\circ\text{C}$$

$$\lambda = 0.4251 \text{ KJ/gm} = 425.1 \text{ KJ/kg}$$

$$\text{There fore } H_v = 24288 [425.1 + 2.41 (42.1 - 25)]$$

$$= 11.3257 \times 10^6 \text{ KJ/hr}$$

$$H_D = DC_p(T_b - T_0)$$

$$= 16192 \times 2.41 (42.1 - 25)$$

$$= 6.673 \times 10^5 \text{ KJ/hr}$$

$$H_L = L C_p (T_b - T_0)$$

$$= 8096 \times 2.41 (42.1 - 25)$$

$$= 3.336 \times 10^5 \text{ KJ/hr}$$

Taking enthalpy balance around the condenser,

$$H_v = Q_c + H_D + H_L$$

$$11.3257 \times 10^6 = Q_c + 6.675 \times 10^5 + 3.336 \times 10^5$$

$$Q_c = 10.325 \times 10^6 \text{ KJ/hr}$$

Cooling water requirement :

Let us assume inlet and exit water temperature as 25°C and 45°C

$$C_p = 4.18 \text{ KJ/kg }^\circ\text{C}$$

$$\text{There fore } Q_c = m_{\text{steam}} C_p \Delta T$$

$$10.325 \times 10^6 = m_{\text{steam}} \times 4.18 \times 20$$

$$m = 123.5 \times 10^3 \text{ kg/hr}$$

Total enthalpy balance :

$$H_F + Q_B = H_D + Q_C + H_W$$

To find H_w :

$$H_w = W C_p \text{ avg } (T_b - T_0)$$

By using $p_i = X_i P_t$ and checking $P_t = 760 \text{ mm Hg}$ we found $T_b = 137^\circ\text{C}$

$$C_p \text{ avg} = 0.776 \times 176.32 + 0.01199 \times 257.11 + 0.2120 \times 110.73$$

$$= 174 \text{ J/mole K}$$

$$= 174 \text{ kJ/kmole K}$$

$$M_{\text{avg}} = 111.72 \text{ kg/kmole}$$

Therefore $C_p \text{ avg} = 174 / 111.72$

$$= 1.5575 \text{ KJ/kg K}$$

$$H_w = 1381.72 \times 1.5575(137-25) \times 111.72$$

$$= 26.927 \times 10^6 \text{ KJ/hr}$$

$H_F = 0$ [because $T_F = T_0$]

$$Q_B = H_D + Q_C + H_w - H_F$$

$$= 6.673 \times 10^5 + 10.325 \times 10^6 + 26.927 \times 10^6 - 0$$

$$= 37.92 \times 10^6 \text{ KJ/hr}$$

Saturated steam required :

$$Q_B = m_{\text{steam}} \lambda$$

$$37.92 \times 10^6 = m_{\text{steam}} \times 2256.9$$

$$m_{\text{steam}} = 16801.5 \text{ kg/hr}$$

Distillation Column – 2 :

$F = 154160 \text{ kg/hr}$ enters at $137 \text{ }^\circ\text{C}$

$D = 15969.4 \text{ kg/hr}$

$W = 138190 \text{ kg/hr}$

Benzene vapor from the top is recycled. Assuming very small propane content to be a part of Benzene stream .

Again assuming $R = 0.5 = L/D$

Hence, $L = 0.5 \times 15969.4 = 7984.7 \text{ kg/hr}$.

$$V = L + D = 167954.1 \text{ kg/hr}$$

Enthalpy of vapor $H_v = V [\lambda + C_p (T_b - T_0)]$

Taking referenced temperature $T_0 = T_F = 137 \text{ }^\circ\text{C}$

B.P. of Benzene at 1 atm = $80.1 \text{ }^\circ\text{C} = T_b$

$$\begin{aligned} \lambda \text{ of Benzene} &= 94.14 \text{ cal /gm} \\ &= 393.8818 \text{ KJ/gm} \\ &= 393.88 \times 10^3 \text{ KJ/kg} \end{aligned}$$

C_p of Benzene vapor at $80.1 \text{ }^\circ\text{C} = 22.83 \text{ cal/gm mole}$

$$\begin{aligned} &= 95.52 \text{ J/gm mole K} \\ &= 1.2246 \text{ KJ/kg } ^\circ\text{K} \end{aligned}$$

$$\begin{aligned} H_v &= 167954.1 [393.8818 + 1.2246 (80.1 - 137)] \\ &= 64.94 \times 10^6 \text{ KJ/hr} \end{aligned}$$

$$\begin{aligned} H_D &= 15969.4 \times 1.2246 (80.1 - 137) \\ &= -1.1127 \times 10^6 \text{ KJ/hr.} \end{aligned}$$

$$\begin{aligned}
H_L &= L C_p (T_b - T_0) \\
&= 7984.7 \times 1.2246 (80.1 - 137) \\
&= -0.55637 \times 10^6 \text{ KJ/hr}
\end{aligned}$$

$$\begin{aligned}
H_v &= Q_C + H_L + H_D \\
54.45 \times 10^6 &= Q_C - 0.55637 \times 10^6 - 1.1127 \times 10^6 \\
Q_C &= 56.12 \times 10^6 \text{ KJ/hr}
\end{aligned}$$

Cooling water requirement :

Let us assume inlet and exit water temperature as 25°C and 45 °C

$$C_p = 4.18 \text{ KJ/kg } ^\circ\text{C}$$

There fore $Q_c = m_{\text{steam}} C_p \Delta T$

$$54.45 \times 10^6 = m_{\text{steam}} \times 4.18 \times 20$$

$$m_{\text{steam}} = 67.128 \times 10^4 \text{ kg/hr}$$

Total enthalpy balance :

$$H_F + Q_B = H_V + Q_C + H_w$$

To find H_w :

$$w = 138190 \text{ Kg/hr}$$

$$T_b = T_F \text{ for distillation column } -3$$

$$= 153.4 \text{ } ^\circ\text{C}$$

$$C_p \text{ avg} \approx C_p \text{ of Cumene}$$

$$= 1.91 \text{ KJ/kg } ^\circ\text{C}$$

$$H_w = 138190 \times 1.91(153.4 - 137)$$

$$= 3.0774 \times 10^6 \text{ KJ/hr}$$

$$H_F = 0 \text{ [because } T_F = T_0 \text{]}$$

$$Q_B = 54.94 \times 10^6 + 65.11 \times 10^6 + 4.06 \times 10^6 - 12.245 \times 10^6$$

$$= 11.46 \times 10^7 \text{ KJ/hr}$$

Saturated steam required :

$$Q_B = m_{\text{steam}} \lambda$$

$$11.46 \times 10^7 = m_{\text{steam}} \times 2256.9$$

$$m_{\text{steam}} = 50.81 \times 10^3 \text{ kg/hr}$$

Distillation column – 3 :

$$F = 138190 \text{ kg/hr}$$

$$D = 129051 \text{ kg/hr}$$

$$w = 9139 \text{ kg/hr}$$

Enthalpy of vapor that goes at the top:

As Cumene is the major constituent that goes with the overhead, taking λ and C_p values of Cumene,

$$H_v = V [\lambda + C_p (T_b - T_0)]$$

Taking reference temperature $T_0 = T_F = 153.4 \text{ }^\circ\text{C}$

B.P. of Cumene at 1 atm = 152.4 $^\circ\text{C}$

λ of Cumene = 74.6 cal/gm

$$= 312.1264 \text{ KJ/kg}$$

C_p of Cumene vapor at 152.4 $^\circ\text{C} = 0.4047 \text{ cal/gm } ^\circ\text{K}$

$$= 1.6931 \text{ KJ/kg } ^\circ\text{K}$$

$$V = D + L = 129051 + 68655.1$$

$$=197706.1 \text{ kg/hr}$$

$$H_v = 197706.1 [312.1264 + 1.6931 (152.4 -153.4)]$$

$$= 61.3745 \times 10^6 \text{ KJ/hr}$$

$$H_D = D C_p (T_b -T_0)$$

$$= 129051 \times 1.6931(152.4 -153.4)$$

$$= -0.218496 \times 10^6 \text{ KJ/hr}$$

$$H_L = L C_p(T_b -T_0)$$

$$= 68655.1 \times 1.6931(152.4 -153.4)$$

$$= -0.116239 \times 10^6 \text{ KJ/hr}$$

$$H_v = Q_C + H_D + H_L$$

$$61.3745 \times 10^6 = Q_C -0.218496 \times 10^6 -0.116239 \times 10^6$$

$$Q_C = 61.71 \times 10^6 \text{ KJ/hr}$$

Cooling water requirement :

Let us assume inlet and exit water temperature as 25°C and 45 °C

$$C_p=4.18 \text{ KJ/kg } ^\circ\text{C}$$

There fore $Q_c = m_{\text{steam}} C_p dT$

$$61.71 \times 10^6 = m_{\text{steam}} \times 4.18 \times 20$$

$$m_{\text{steam}} = 73.8148 \times 10^3 \text{ kg/hr}$$

Total enthalpy balance :

$$H_F + Q_B = H_V + Q_C + H_w$$

To find H_w :

$$W = 9139 \text{ kg/hr}$$

$$H_w = W C_p \text{ avg } (T_b -T_0)$$

$$T_b \text{ at } x_w = 0.2934 = 184.5 \text{ } ^\circ\text{C}$$

$$\begin{aligned} C_p \text{ avg at } 184.5 \text{ } ^\circ\text{C} &= 0.013 \times 214.1952 + (1 - 0.013) \times 288.93 \\ &= 287.9584 \text{ J/mole } ^\circ\text{K} \\ &= 2.88795 \text{ KJ/kg } ^\circ\text{K} \end{aligned}$$

$$\begin{aligned} H_w &= 9139 \times 2.8795(184.5 - 153.4) \\ &= 81.84 \times 10^4 \text{ KJ/hr} \end{aligned}$$

$$H_F = 0 \text{ [because } T_F = T_0 \text{]}$$

$$\begin{aligned} Q_B &= H_V + Q_C + H_W - H_F \\ &= 61.3745 \times 10^6 + 73.8143 \times 10^3 + 81.84 \times 10^4 \\ &= 62.2667 \times 10^6 \text{ KJ/hr} \end{aligned}$$

Saturated steam required :

$$\begin{aligned} Q_B &= m_{\text{steam}} \lambda \\ 62.2667 \times 10^6 &= m_{\text{steam}} \times 2256.9 \\ m_{\text{steam}} &= 27589.5 \text{ kg/hr} \end{aligned}$$