

## ENERGY BALANCE

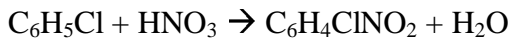
Component	Melting point ( $^{\circ}\text{C}$ )	Boiling point ( $^{\circ}\text{C}$ )
Para Isomer	83	242 $^{\circ}\text{C}$ at 101 Kpa 113 $^{\circ}\text{C}$ at 1.1 Kpa
Meta Isomer	46	235.6 at 101 Kpa
Ortho Isomer	32.5	245.5 at 101 Kpa 119 at 1.1 Kpa

Density of para Isomer = 1.520 gm/cc

Density of ortho isomer = 1.368 gm/cc

Density of meta Isomer = 1.534 gm/cc

Melting point of para Isomer is highest hence it deposits crystals first upon cooling.



Heat of formation, H = Heat of formation of ( $\text{C}_a\text{H}_b\text{Br}_c$ )

From group contribution method,

Value of H is = 143 kJ/mol.

Value of C is = 390 kJ/mol

Value of NO<sub>2</sub> is = - 33 KJ/mol.

∴ Heat of formation

$$H = [-Q + 390a + 143b] \text{KJ/mol}$$

$$Q(\text{HNO}_3) = 104.5 \text{ KJ/mol}$$

$$Q(\text{C}_6\text{H}_5\text{Cl}) = 3218 \text{ KJ/mol}$$

$$Q(\text{H}_2\text{O}) = 284 \text{ KJ/mol}$$

$$\begin{aligned} H(\text{C}_6\text{H}_5\text{Cl}) &= -3218 + 390 \times 6 + 143 \times 5 \\ &= -140.9 \text{ KJ / mol} \end{aligned}$$

$$H(\text{C}_6\text{H}_5\text{ClNO}_2) = -2708.64 + 390 \times 6 + 143 \times 4$$

$$= 240.33 \text{ KJ/mol}$$

$$H(\text{H}_2\text{O}) = -28.25 \text{ KJ / hr}$$

$$H(\text{HNO}_3) = -206.62 \text{ KJ / hr.}$$

Heat of Reaction

$$H_R = H (\text{products}) - H (\text{Reactant})$$

$$= [ -240.33 - 284.25 ] - [ 140.9 - 206.62 ]$$

$$= - 179.25 \text{ KJ per mole of chlorobenzene nitrated.}$$

## **PREDICTION OF SPECIFIC HEAT VALUES**

From Perry chemical engineering hand book (6<sup>th</sup> edition).

Heat capacity of chlorobenzene = 1.38 KJ / kg °C

## **HEAT CAPACITY OF NITROCHLOROBENZENE**

From group contribution method.

$C_p$ [Nitrochlorobenzene]

$$= 6 \times 7.5 + 4 \times 18 + 33.5 \times 33.5 + 2 \times 25.1$$

$$= 234.2 \text{ J/gr mole}$$

$$= \frac{234.2}{157.5} \text{ J / gm}^{\circ}\text{C}$$

$$= 1486 \text{ KJ / Kg}^{\circ}\text{C}$$

## **Jet mixer of acids:**

Basis: 1 hour of operation.

Heat is evolved when nitric acid and sulphuric acids are mixed together and the temperature raise can be large. The heat liberated in mixing may be determined from the chart developed by Mecerdy & Kinley from the experimental data of Rhodes and Nelson.

(Cremer chemical engineering practice volume 1).

**Relative enthalpy**

Nitric acid	90%	- 87BTU/lb =-199.8 KJ/kg
Sulphuric acid	96%	-82.1 KJ/kg

**Input to the mixer:**

	Weight (Kg)	Heat KJ
Sulphuric acid	395	32429.5
Nitric acid	284.8	56903.04

**Output from the mixer:**

	Relative enthalpy	Weight	Heat content
Mixed acid	-170 (KJ/kg)	679.8	-115566

Therefore heat evolved on mixing

$$= - 1115566 + 89332.54$$

$$= - 26233.41 \text{ KJ/hr.}$$

(Heat evolved in forming, 1 kg of mixed acid)

Temperature raise,  $= \frac{\text{-----}}{\text{Specific heat of acid.}}$

Heat capacity of acid  $= 0.44 \times 4186$   
 $= 1841.84 \text{ KJ}$

Therefore temperature raise  $= \frac{26233.41 \times 10^3}{679 \times 1841.64}$

$$= 21^{\circ}\text{C}$$

∴ If acid enters at 23<sup>0</sup>C their outlet temperature will be = 44<sup>0</sup>C

## NITRATOR

Reaction in the nitrator is carried out at 50<sup>0</sup>C

Heat of reaction, H<sub>R</sub> = - 179.24 KJ per mole of chlorobenzene nitrated.

$$= - 179.24 \times 457.867$$

$$= - 94282.1 \text{ KJ/hr}$$

Temperature to be maintained in the reactor is 50<sup>0</sup>C

Inlet temperature of chlorobenzene = 23<sup>0</sup>C

Inlet Temperature of mixed acid = 44<sup>0</sup>C

Heat absorbed by mixed acid,

$$= (50-44) \times 0.44 \times 4.187 \times 679.8$$

$$= 7514.29 \text{ KJ/hr}$$

Heat capacity of chlorobenzene

$$= 0.33 \text{ BTU/lb}^{\circ}\text{F}$$

Heat absorbed by chlorobenzene

$$= 467.62 \times 0.33 \times 4.18 \times (50-23)$$

$$= 17416 \text{ KJ/hr}$$

Heat to be removed by cooling water

$$= 94282.1 - 7514.29 - 17416$$

$$= 69352 \text{ KJ/hr}$$

Assuming temperature raise of cooling water to be equal to 10<sup>0</sup>C.

Therefore quantity of cooling water required

$$= \frac{69352 \times 10^3}{4.187 \times 10^3 \times 10}$$

$$= 16456.34 \text{ kg./hr}$$

Sensible heat above datum of spent acid

$$= 498.5 \times 0.44 \times 4187 \times (50 - 23)$$

$$= 24796.6 \text{ KJ/hr}$$

## Washing process

After separation of mononitrated chlorobenzene the solution is washed with  $\text{Na}_2\text{CO}_3$  and then water, the washing is carried out continuously with counter current flow in Holley – Mott washer.

Water flow rate = 1300.46 kg/hr (at  $23^\circ\text{C}$ )

Sodium carbonate flow rate = 3.28 kg/hr (at  $23^\circ\text{C}$ )

Heat in mono nitrochlorobenzene above datum

$$= 641.01 \times 1.486 \times (50 - 23)$$

$$= 25718 \text{ KJ/hr}$$

All the heat is transferred to wash solution.

Temperature raise of wash solution

$$= \frac{25718 \times 10^3}{(1300.46 + 3.28)} \times \frac{1}{4187}$$

$$= 4.7^\circ\text{C}$$

## CRYSTALLIZER HEAT BALANCE

### 1<sup>ST</sup> CRYSTALLIZER

The para Isomer crystallizes at  $16^\circ\text{C}$ . Mononitrochlorobenzene stream comes at a temperature of  $23^\circ\text{C}$  to the crystallizer

Flow rate of nitrated product

$$= 641.01 \text{ kg/hr}$$

Specific heat of mononitrochlorobenzene

$$= 1486 \text{ J /kg}^\circ\text{C}$$

Specific heat of brine solution (25% NaCl)

$$= 3391.47 \text{ J/Kg}^0\text{C}$$

Heat to be absorbed by brine

$$= 641.01 \times 1486 \times (23-15)$$

$$= 7620 \text{ KJ/hr}$$

Assume that brine solution enters at  $-5^0\text{C}$ , and temperature raise of brine solution to be  $10^0\text{C}$ ,

$$\begin{aligned} \text{Flow rate of brine required} &= \frac{Q}{C_p \Delta t} \\ &= \frac{7620 \times 10^3}{3391 \times 10} \\ &= 224 \text{ kg/hr} \end{aligned}$$

## 2<sup>nd</sup> crystallizer

Here crystallization takes place at a temperature of  $18^0\text{C}$

Mononitrochlorobenzene enters the crystallizer at a temperature of  $214.541^0\text{C}$

Flow rate of Nitrated product

$$= 3309 \text{ kg/hr}$$

Specific heat of Mononitrochlorobenzene

$$= 1.486 \text{ KJ/kg}^0\text{C}$$

Heat to be absorbed by the brine solution, Q

$$= 3309 \times 1.486 \times (214.54 - 18)$$

$$= 966.426 \times 10^3 \text{ KJ / hr}$$

Let entering temperature of brine solution is equal to  $-5^0\text{C}$  assuming temperature raise of  $25^0\text{C}$  of brine solution.

Then amount of brine required

$$\begin{aligned} M &= \frac{966.426 \times 10^3}{3.391 \times 25} \\ &= 11.39 \times 10^3 \text{ kg/hr} \\ &= 3.16 \text{ kg/sec} \end{aligned}$$

## Heat balance for condenser

Latent heat of vaporization of Nitrated product  $\lambda = 338.03 \text{ KJ/kg}$ .

Mass flow rate of nitrated product to be condensed

$$M = 0.919 \text{ kg/sec}$$

Therefore amount of heat to be removed  $= m\lambda$

$$= 338.03 \times 0.919$$

$$= 310.65 \text{ KJ/sec}$$

Let cooling water enter at  $30^{\circ}\text{C}$ . Assuming temperature raise of cooling water to be  $10^{\circ}\text{C}$ .

Therefore temperature of cooling water at the outlet  $= 40^{\circ}\text{C}$

Amount of cooling water required  $Q = M_w C_p \Delta t$

$$310.65 \times 10^3 = M_w \times 4.18 \times 10^3 \times 10$$

$$M_w = 7.43 \text{ kg / sec}$$